making it impossible to reach colossal patterns. Even depth-first search methods like FP-growth can be easily trapped in a huge amount of subtrees before reaching colossal patterns. Clearly, a completely new mining methodology is needed to overcome such a hurdle.

A new mining strategy called *Pattern-Fusion* was developed, which fuses a small number of shorter frequent patterns into colossal pattern candidates. It thereby takes leaps in the pattern search space and avoids the pitfalls of both breadth-first and depth-first searches. This method finds a good approximation to the complete set of *colossal* frequent patterns.

The Pattern-Fusion method has the following major characteristics. First, it traverses the tree in a bounded-breadth way. Only a fixed number of patterns in a bounded-size candidate pool are used as starting nodes to search downward in the pattern tree. As such, it avoids the problem of exponential search space.

Second, Pattern-Fusion has the capability to identify "shortcuts" whenever possible. Each pattern's growth is not performed with one-item addition, but with an agglomeration of multiple patterns in the pool. These shortcuts direct Pattern-Fusion much more rapidly down the search tree toward the colossal patterns. Figure 7.8 conceptualizes this mining model.

As Pattern-Fusion is designed to give an approximation to the colossal patterns, a quality evaluation model is introduced to assess the patterns returned by the algorithm. An empirical study verifies that Pattern-Fusion is able to efficiently return high-quality results.

Let's examine the Pattern-Fusion method in more detail. First, we introduce the concept of **core pattern**. For a pattern α, an itemset $\beta \subseteq \alpha$ is said to be a τ*-core pattern* of α if $\frac{|D_\alpha|}{|D_\beta|} \geq \tau$, $0 < \tau \leq 1$, where $|D_\alpha|$ is the number of patterns containing α in database

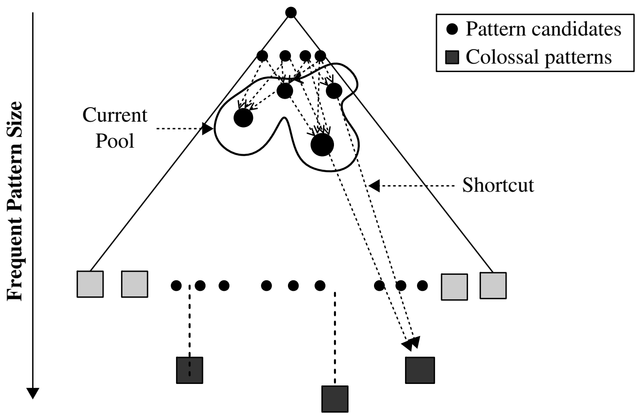

Figure 7.8 Pattern tree traversal: Candidates are taken from a pool of patterns, which results in shortcuts through pattern space to the colossal patterns.

D. τ is called the *core ratio*. A pattern α is *(d,τ)-robust* if d is the maximum number of items that can be removed from α for the resulting pattern to remain a τ-core pattern of α, that is,

$$d = \max_{\beta}\{|\alpha| - |\beta| \,|\, \beta \subseteq \alpha, \text{ and } \beta \text{ is a } \tau\text{-core pattern of } \alpha\}.$$

Example 7.11 **Core patterns.** Figure 7.9 shows a simple transaction database of four distinct transactions, each with 100 duplicates: $\{\alpha_1 = (abe),\ \alpha_2 = (bcf),\ \alpha_3 = (acf),\ \alpha_4 = (abcfe)\}$. If we set $\tau = 0.5$, then (ab) is a core pattern of α_1 because (ab) is contained only by α_1 and α_4. Therefore, $\frac{|D_{\alpha_1}|}{|D_{(ab)}|} = \frac{100}{200} \geq \tau$. α_1 is $(2, 0.5)$-robust while α_4 is $(4, 0.5)$-robust. The table also shows that larger patterns (e.g., $(abcfe)$) have far more core patterns than smaller ones (e.g., (bcf)). ■

From Example 7.11, we can deduce that large or colossal patterns have far more core patterns than smaller patterns do. Thus, a colossal pattern is more robust in the sense that *if a small number of items are removed from the pattern, the resulting pattern would have a similar support set.* The larger the pattern size, the more prominent this robustness. Such a robustness relationship between a colossal pattern and its corresponding core patterns can be extended to multiple levels. The lower-level core patterns of a colossal pattern are called **core descendants**.

Given a small c, a colossal pattern usually has far more core descendants of size c than a smaller pattern. This means that if we were to draw randomly from the complete set of patterns of size c, we would be more likely to pick a core descendant of a colossal pattern than that of a smaller pattern. In Figure 7.9, consider the complete set of patterns of size $c = 2$, which contains $\binom{5}{2} = 10$ patterns in total. For illustrative purposes, let's assume that the larger pattern, *abcef*, is colossal. The probability of being able to randomly draw a core descendant of *abcef* is 0.9. Contrast this to the probability of randomly drawing a core descendent of smaller (noncolossal) patterns, which is at most 0.3. Therefore, a colossal pattern can be generated by merging a proper set of

Transactions (# of Transactions)	*Core Patterns* ($\tau = 0.5$)
(abe) (100)	(abe), (ab), (be), (ae), (e)
(bcf) (100)	(bcf), (bc), (bf)
(acf) (100)	(acf), (ac), (af)
$(abcef)$ (100)	(ab), (ac), (af), (ae), (bc), (bf), (be), (ce), (fe), (e), (abc), (abf), (abe), (ace), (acf), (afe), (bcf), (bce), (bfe), (cfe), $(abcf)$, $(abce)$, $(bcfe)$, $(acfe)$, $(abfe)$, $(abcef)$

Figure 7.9 A transaction database, which contains duplicates, and core patterns for each distinct transaction.

its core patterns. For instance, *abcef* can be generated by merging just two of its core patterns, *ab* and *cef*, instead of having to merge all of its 26 core patterns.

Now, let's see how these observations can help us leap through pattern space more directly toward colossal patterns. Consider the following scheme. First, generate a complete set of frequent patterns up to a user-specified small size, and then randomly pick a pattern, β. β will have a high probability of being a core-descendant of some colossal pattern, α. Identify all of α's core-descendants in this complete set, and merge them. This generates a much larger core-descendant of α, giving us the ability to leap along a path toward α in the core-pattern tree, T_α. In the same fashion we select K patterns. The set of larger core-descendants generated is the candidate pool for the next iteration.

A question arises: Given β, a core-descendant of a colossal pattern α, how can we find the other core-descendants of α? Given two patterns, α and β, the pattern distance between them is defined as $Dist(\alpha, \beta) = 1 - \frac{|D_\alpha \cap D_\beta|}{|D_\alpha \cup D_\beta|}$. Pattern distance satisfies the triangle inequality.

For a pattern, α, let C_α be the set of all its core patterns. It can be shown that C_α is bounded in metric space by a "ball" of diameter $r(\tau)$, where $r(\tau) = 1 - \frac{1}{2/\tau - 1}$. This means that given a core pattern $\beta \in C_\alpha$, we can identify all of α's core patterns in the current pool by posing a range query. Note that in the mining algorithm, each randomly drawn pattern could be a core-descendant of more than one colossal pattern, and as such, when merging the patterns found by the "ball," more than one larger core-descendant could be generated.

From this discussion, the Pattern-Fusion method is outlined in the following two phases:

1. **Initial Pool:** Pattern-Fusion assumes an initial pool of small frequent patterns is available. This is the complete set of frequent patterns up to a small size (e.g., 3). This initial pool can be mined with any existing efficient mining algorithm.
2. **Iterative Pattern-Fusion:** Pattern-Fusion takes as input a user-specified parameter, K, which is the maximum number of patterns to be mined. The mining process is iterative. At each iteration, K seed patterns are randomly picked from the current pool. For each of these K seeds, we find all the patterns within a ball of a size specified by τ. All the patterns in each "ball" are then fused together to generate a set of superpatterns. These superpatterns form a new pool. If the pool contains more than K patterns, the next iteration begins with this pool for the new round of random drawing. As the support set of every superpattern shrinks with each new iteration, the iteration process terminates.

Note that *Pattern-Fusion merges small subpatterns of a large pattern instead of incrementally-expanding patterns with single items.* This gives the method an advantage to circumvent midsize patterns and progress on a path leading to a potential colossal pattern. The idea is illustrated in Figure 7.10. Each point shown in the metric space

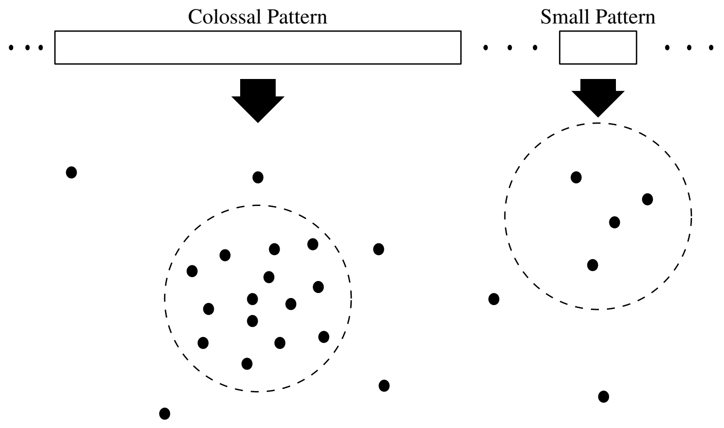

Figure 7.10 Pattern metric space: Each point represents a core pattern. The core patterns of a colossal pattern are denser than those of a small pattern, as shown within the dotted lines.

represents a core pattern. In comparison to a smaller pattern, a larger pattern has far more core patterns that are close to one another, all of which are bounded by a ball, as shown by the dotted lines. When drawing randomly from the initial pattern pool, we have a much higher probability of getting a core pattern of a large pattern, because the ball of a larger pattern is much denser.

It has been theoretically shown that Pattern-Fusion leads to a good approximation of colossal patterns. The method was tested on synthetic and real data sets constructed from program tracing data and microarray data. Experiments show that the method can find most of the colossal patterns with high efficiency.

7.5 Mining Compressed or Approximate Patterns

A major challenge in frequent pattern mining is the huge number of discovered patterns. Using a minimum support threshold to control the number of patterns found has limited effect. Too low a value can lead to the generation of an explosive number of output patterns, while too high a value can lead to the discovery of only commonsense patterns.

To reduce the huge set of frequent patterns generated in mining while maintaining high-quality patterns, we can instead mine a compressed or approximate set of frequent patterns. *Top-k most frequent closed patterns* were proposed to make the mining process concentrate on only the set of *k* most frequent patterns. Although interesting, they usually do not epitomize the *k* most representative patterns because of the uneven frequency distribution among itemsets. *Constraint-based mining* of frequent patterns (Section 7.3) incorporates user-specified constraints to filter out uninteresting patterns. Measures of pattern/rule *interestingness* and *correlation* (Section 6.3) can also be used to help confine the search to patterns/rules of interest.

In this section, we look at two forms of "compression" of frequent patterns that build on the concepts of closed patterns and max-patterns. Recall from Section 6.2.6 that a *closed pattern* is a lossless compression of the set of frequent patterns, whereas a *max-pattern* is a lossy compression. In particular, Section 7.5.1 explores *clustering-based compression of frequent patterns*, which groups patterns together based on their similarity and frequency support. Section 7.5.2 takes a "*summarization*" *approach*, where the aim is to derive redundancy-aware top-k representative patterns that cover the whole set of (closed) frequent itemsets. The approach considers not only the representativeness of patterns but also their mutual independence to avoid redundancy in the set of generated patterns. The k representatives provide compact compression over the collection of frequent patterns, making them easier to interpret and use.

7.5.1 Mining Compressed Patterns by Pattern Clustering

Pattern compression can be achieved by pattern clustering. Clustering techniques are described in detail in Chapters 10 and 11. In this section, it is not necessary to know the fine details of clustering. Rather, you will learn how the concept of clustering can be applied to compress frequent patterns. Clustering is the automatic process of grouping like objects together, so that objects within a cluster are similar to one another and dissimilar to objects in other clusters. In this case, the objects are frequent patterns. The frequent patterns are clustered using a tightness measure called δ-cluster. A representative pattern is selected for each cluster, thereby offering a compressed version of the set of frequent patterns.

Before we begin, let's review some definitions. An itemset X is a **closed frequent itemset** in a data set D if X is frequent and there exists no proper super-itemset Y of X such that Y has the same support count as X in D. An itemset X is a **maximal frequent itemset** in data set D if X is frequent and there exists no super-itemset Y such that $X \subset Y$ and Y is frequent in D. Using these concepts alone is not enough to obtain a good representative compression of a data set, as we see in Example 7.12.

Example 7.12 **Shortcomings of closed itemsets and maximal itemsets for compression.** Table 7.3 shows a subset of frequent itemsets on a large data set, where *a, b, c, d, e, f* represent individual items. There are no closed itemsets here; therefore, we cannot use closed frequent itemsets to compress the data. The only maximal frequent itemset is P_3. However, we observe that itemsets P_2, P_3, and P_4 are significantly different with respect to their support counts. If we were to use P_3 to represent a compressed version of the data, we would lose this support count information entirely. From visual inspection, consider the two pairs (P_1, P_2) and (P_4, P_5). The patterns within each pair are very similar with respect to their support and expression. Therefore, intuitively, P_2, P_3, and P_4, collectively, should serve as a better compressed version of the data. ■

Table 7.3 Subset of Frequent Itemsets

ID	*Itemsets*	*Support*
P_1	$\{b, c, d, e\}$	205,227
P_2	$\{b, c, d, e, f\}$	205,211
P_3	$\{a, b, c, d, e, f\}$	101,758
P_4	$\{a, c, d, e, f\}$	161,563
P_5	$\{a, c, d, e\}$	161,576

So, let's see if we can find a way of clustering frequent patterns as a means of obtaining a compressed representation of them. We will need to define a good similarity measure, cluster patterns according to this measure, and then select and output only a *representative pattern* for each cluster. Since the set of closed frequent patterns is a lossless compression over the original frequent patterns set, it is a good idea to discover representative patterns over the collection of *closed* patterns.

We can use the following distance measure between closed patterns. Let P_1 and P_2 be two closed patterns. Their supporting transaction sets are $T(P_1)$ and $T(P_2)$, respectively. The **pattern distance** of P_1 and P_2, $Pat\_Dist(P_1, P_2)$, is defined as

$$Pat\_Dist(P_1, P_2) = 1 - \frac{|T(P_1) \cap T(P_2)|}{|T(P_1) \cup T(P_2)|}. \tag{7.14}$$

Pattern distance is a valid distance metric defined on the set of transactions. Note that it incorporates the *support* information of patterns, as desired previously.

Example 7.13 **Pattern distance.** Suppose P_1 and P_2 are two patterns such that $T(P_1) = \{t_1, t_2, t_3, t_4, t_5\}$ and $T(P_2) = \{t_1, t_2, t_3, t_4, t_6\}$, where t_i is a transaction in the database. The distance between P_1 and P_2 is $Pat\_Dist(P_1, P_2) = 1 - \frac{4}{6} = \frac{1}{3}$. ■

Now, let's consider the *expression* of patterns. Given two patterns A and B, we say B can be **expressed** by A if $O(B) \subset O(A)$, where $O(A)$ is the corresponding itemset of pattern A. Following this definition, assume patterns $P_1, P_2, \ldots, P_k$ are in the same cluster. The representative pattern P_r of the cluster should be able to *express* all the other patterns in the cluster. Clearly, we have $\cup_{i=1}^{k} O(P_i) \subseteq O(P_r)$.

Using the distance measure, we can simply apply a clustering method, such as k-means (Section 10.2), on the collection of frequent patterns. However, this introduces two problems. First, the quality of the clusters cannot be guaranteed; second, it may not be able to find a representative pattern for each cluster (i.e., the pattern P_r may not belong to the same cluster). To overcome these problems, this is where the concept of δ-cluster comes in, where δ $(0 \leq \delta \leq 1)$ measures the tightness of a cluster.

A pattern P is **δ-covered** by another pattern P' if $O(P) \subseteq O(P')$ and $Pat\_Dist(P, P') \leq \delta$. A set of patterns form a **δ-cluster** if there exists a representative pattern P_r such that for each pattern P in the set, P is δ-covered by P_r.

Note that according to the concept of δ-cluster, a pattern can belong to multiple clusters. Also, using δ-cluster, we only need to compute the distance between each pattern and the representative pattern of the cluster. Because a pattern P is δ-covered by a representative pattern P_r only if $O(P) \subseteq O(P_r)$, we can simplify the distance calculation by considering only the supports of the patterns:

$$Pat\_Dist(P, P_r) = 1 - \frac{|T(P) \cap T(P_r)|}{|T(P) \cup T(P_r)|} = 1 - \frac{|T(P_r)|}{|T(P)|}. \tag{7.15}$$

If we restrict the representative pattern to be frequent, then the number of representative patterns (i.e., clusters) is no less than the number of maximal frequent patterns. This is because a maximal frequent pattern can only be covered by itself. To achieve more succinct compression, we relax the constraints on representative patterns, that is, we allow the support of representative patterns to be *somewhat* less than *min_sup*.

For any representative pattern P_r, assume its support is k. Since it has to *cover* at least one frequent pattern (i.e., P) with support that is at least *min_sup*, we have

$$\delta \geq Pat\_Dist(P, P_r) = 1 - \frac{|T(P_r)|}{|T(P)|} \geq 1 - \frac{k}{min\_sup}. \tag{7.16}$$

That is, $k \geq (1 - \delta) \times min\_sup$. This is the minimum support for a representative pattern, denoted as min_sup_r.

Based on the preceding discussion, the pattern compression problem can be defined as follows: *Given a transaction database, a minimum support* min_sup, *and the cluster quality measure* δ, *the pattern compression problem is to find a set of representative patterns* R *such that for each frequent pattern* P *(with respect to* min_sup), *there is a representative pattern* $P_r \in R$ *(with respect to* min_sup_r), *which covers* P, *and the value of* $|R|$ *is minimized.*

Finding a minimum set of representative patterns is an NP-Hard problem. However, efficient methods have been developed that reduce the number of closed frequent patterns generated by orders of magnitude with respect to the original collection of closed patterns. The methods succeed in finding a high-quality compression of the pattern set.

7.5.2 Extracting Redundancy-Aware Top-*k* Patterns

Mining the top-k most frequent patterns is a strategy for reducing the number of patterns returned during mining. However, in many cases, frequent patterns are not mutually independent but often clustered in small regions. This is somewhat like finding 20 population centers in the world, which may result in cities clustered in a small number of countries rather than evenly distributed across the globe. Instead, most users would prefer to derive the k most interesting patterns, which are not only significant, but also mutually independent and containing little redundancy. A small set of

k representative patterns that have not only high significance but also low redundancy are called **redundancy-aware top-*k* patterns**.

Example 7.14 **Redundancy-aware top-*k* strategy versus other top-*k* strategies.** Figure 7.11 illustrates the intuition behind *redundancy-aware top-k patterns* versus *traditional top-k patterns* and *k-summarized patterns.* Suppose we have the frequent patterns set shown in Figure 7.11(a), where each circle represents a pattern of which the significance is colored in grayscale. The distance between two circles reflects the redundancy of the two corresponding patterns: The closer the circles are, the more redundant the respective patterns are to one another. Let's say we want to find three patterns that will best represent the given set, that is, $k = 3$. Which three should we choose?

Arrows are used to show the patterns chosen if using redundancy-aware top-k patterns (Figure 7.11b), traditional top-k patterns (Figure 7.11c), or k-summarized patterns (Figure 7.11d). In Figure 7.11(c), the **traditional top-*k* strategy** relies solely on significance: It selects the three most significant patterns to represent the set.

In Figure 7.11(d), the ***k*-summarized pattern strategy** selects patterns based solely on nonredundancy. It detects three clusters, and finds the most representative patterns to

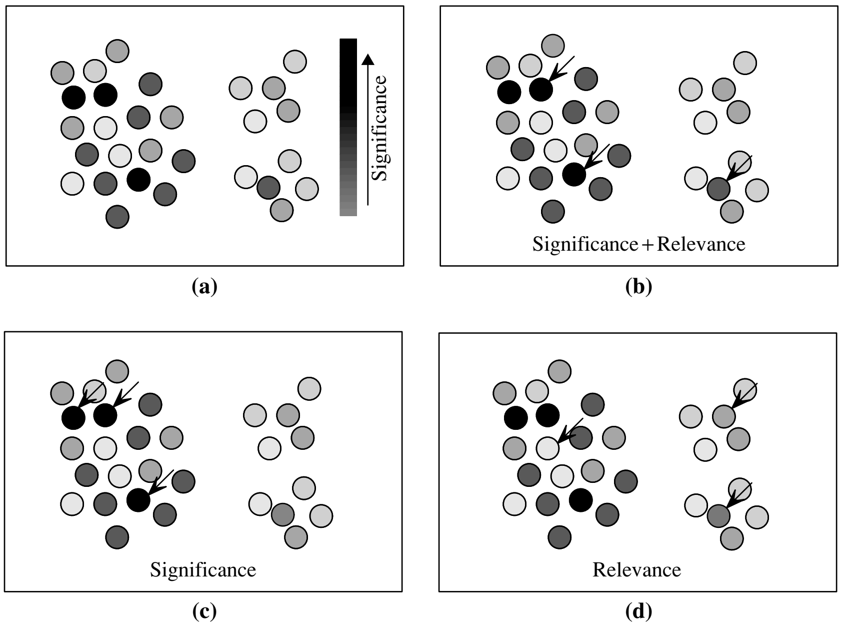

Figure 7.11 Conceptual view comparing top-k methodologies (where gray levels represent pattern significance, and the closer that two patterns are displayed, the more redundant they are to one another): (a) original patterns, (b) redundancy-aware top-k patterns, (c) traditional top-k patterns, and (d) k-summarized patterns.

be the "centermost'" pattern from each cluster. These patterns are chosen to represent the data. The selected patterns are considered "summarized patterns" in the sense that they represent or "provide a summary" of the clusters they stand for.

By contrast, in Figure 7.11(d) the **redundancy-aware top-*k* patterns** make a trade-off between significance and redundancy. The three patterns chosen here have high significance and low redundancy. Observe, for example, the two highly significant patterns that, based on their redundancy, are displayed next to each other. The redundancy-aware top-k strategy selects only one of them, taking into consideration that two would be redundant. To formalize the definition of redundancy-aware top-k patterns, we'll need to define the concepts of significance and redundancy. ■

A **significance measure** S is a function mapping a pattern $p \in \mathcal{P}$ to a real value such that $S(p)$ is the degree of interestingness (or usefulness) of the pattern p. In general, significance measures can be either objective or subjective. *Objective measures* depend only on the structure of the given pattern and the underlying data used in the discovery process. Commonly used objective measures include support, confidence, correlation, and *tf-idf* (or *term frequency* versus *inverse document frequency*), where the latter is often used in information retrieval. *Subjective* measures are based on user beliefs in the data. They therefore depend on the users who examine the patterns. A subjective measure is usually a relative score based on user prior knowledge or a background model. It often measures the unexpectedness of a pattern by computing its divergence from the background model. Let $S(p,q)$ be the **combined significance** of patterns p and q, and $S(p|q) = S(p,q) - S(q)$ be the **relative significance** of p given q. Note that the combined significance, $S(p,q)$, means the collective significance of two individual patterns p and q, not the significance of a single super pattern $p \cup q$.

Given the significance measure S, the **redundancy** R **between two patterns** p and q is defined as $R(p,q) = S(p) + S(q) - S(p,q)$. Subsequently, we have $S(p|q) = S(p) - R(p,q)$.

We assume that the combined significance of two patterns is no less than the significance of any individual pattern (since it is a collective significance of two patterns) and does not exceed the sum of two individual significance patterns (since there exists redundancy). That is, the redundancy between two patterns should satisfy

$$0 \le R(p,q) \le \min(S(p), S(q)). \tag{7.17}$$

The ideal redundancy measure $R(p,q)$ is usually hard to obtain. However, we can approximate redundancy using distance between patterns such as with the distance measure defined in Section 7.5.1.

The problem of finding redundancy-aware top-k patterns can thus be transformed into finding a k-pattern set that maximizes the marginal significance, which is a well-studied problem in information retrieval. In this field, a document has high marginal relevance if it is both relevant to the query and contains minimal marginal similarity to previously selected documents, where the marginal similarity is computed by choosing the most relevant selected document. Experimental studies have shown this method to be efficient and able to find high-significance and low-redundancy top-k patterns.

7.6 Pattern Exploration and Application

For discovered frequent patterns, is there any way the mining process can return additional information that will help us to better understand the patterns? What kinds of applications exist for frequent pattern mining? These topics are discussed in this section. Section 7.6.1 looks at the automated generation of **semantic annotations** for frequent patterns. These are dictionary-like annotations. They provide semantic information relating to patterns, based on the context and usage of the patterns, which aids in their understanding. Semantically similar patterns also form part of the annotation, providing a more direct connection between discovered patterns and any other patterns already known to the users.

Section 7.6.2 presents an overview of applications of frequent pattern mining. While the applications discussed in Chapter 6 and this chapter mainly involve market basket analysis and correlation analysis, there are many other areas in which frequent pattern mining is useful. These range from data preprocessing and classification to clustering and the analysis of complex data.

7.6.1 Semantic Annotation of Frequent Patterns

Pattern mining typically generates a huge set of frequent patterns without providing enough information to interpret the meaning of the patterns. In the previous section, we introduced pattern processing techniques to shrink the size of the output set of frequent patterns such as by extracting redundancy-aware top-k patterns or compressing the pattern set. These, however, do not provide any semantic interpretation of the patterns. It would be helpful if we could also generate semantic annotations for the frequent patterns found, which would help us to better understand the patterns.

"*What is an appropriate semantic annotation for a frequent pattern?*" Think about what we find when we look up the meaning of terms in a dictionary. Suppose we are looking up the term *pattern*. A dictionary typically contains the following components to explain the term:

1. *A set of definitions*, such as "a decorative design, as for wallpaper, china, or textile fabrics, etc.; a natural or chance configuration"
2. *Example sentences*, such as "*patterns* of frost on the window; the behavior *patterns* of teenagers, ..."
3. *Synonyms from a thesaurus*, such as "model, archetype, design, exemplar, motif, ..."

Analogically, what if we could extract similar types of semantic information and provide such structured annotations for frequent patterns? This would greatly help users in interpreting the meaning of patterns and in deciding on how or whether to further explore them. Unfortunately, it is infeasible to provide such precise semantic definitions for patterns without expertise in the domain. Nevertheless, we can explore how to *approximate* such a process for frequent pattern mining.

Pattern: "{*frequent, pattern*}"

context indicators:

"mining," "constraint," "Apriori," "FP-growth,"
"rakesh agrawal," "jiawei han," ...

representative transactions:

1) mining *frequent patterns* without candidate ...
2) ... mining closed *frequent* graph *patterns*

semantically similar patterns:

"{*frequent, sequential, pattern*}," "{*graph, pattern*}"
"{*maximal, pattern*}," "{*frequent, closed, pattern*}," ...

Figure 7.12 Semantic annotation of the pattern "{*frequent, pattern*}."

In general, the hidden meaning of a pattern can be inferred from patterns with similar meanings, data objects co-occurring with it, and transactions in which the pattern appears. Annotations with such information are analogous to dictionary entries, which can be regarded as annotating each term with structured semantic information. Let's examine an example.

Example 7.15 **Semantic annotation of a frequent pattern.** Figure 7.12 shows an example of a semantic annotation for the pattern "{*frequent, pattern*}." This dictionary-like annotation provides semantic information related to "{*frequent, pattern*}," consisting of its strongest *context indicators*, the most *representative data transactions*, and the most *semantically similar patterns*. This kind of semantic annotation is similar to natural language processing. The semantics of a word can be inferred from its context, and words sharing similar contexts tend to be semantically similar. The context indicators and the representative transactions provide a view of the context of the pattern from different angles to help users understand the pattern. The semantically similar patterns provide a more direct connection between the pattern and any other patterns already known to the users. ■

"*How can we perform automated semantic annotation for a frequent pattern?*" The key to high-quality semantic annotation of a frequent pattern is the successful context modeling of the pattern. For context modeling of a pattern, p, consider the following.

- A **context unit** is a basic object in a database, D, that carries semantic information and co-occurs with at least one frequent pattern, p, in at least one transaction in D. A context unit can be an item, a pattern, or even a transaction, depending on the specific task and data.
- The **context of a pattern**, p, is a selected set of weighted context units (referred to as **context indicators**) in the database. It carries semantic information, and co-occurs with a frequent pattern, p. The context of p can be modeled using a vector space model, that is, the context of p can be represented as $C(p) = \langle w(u_1),$

$w(u_2), \ldots, w(u_n)\rangle$, where $w(u_i)$ is a weight function of term u_i. A transaction t is represented as a vector $\langle v_1, v_2, \ldots, v_m\rangle$, where $v_i = 1$ if and only if $v_i \in t$, otherwise $v_i = 0$.

Based on these concepts, we can define the basic task of **semantic pattern annotation** as follows:

1. Select context units and design a strength weight for each unit to model the contexts of frequent patterns.
2. Design similarity measures for the contexts of two patterns, and for a transaction and a pattern context.
3. For a given frequent pattern, extract the most significant context indicators, representative transactions, and semantically similar patterns to construct a structured annotation.

"*Which context units should we select as context indicators?*" Although a context unit can be an item, a transaction, or a pattern, typically, frequent patterns provide the most semantic information of the three. There are usually a large number of frequent patterns associated with a pattern, p. Therefore, we need a systematic way to select only the important and nonredundant frequent patterns from a large pattern set.

Considering that the closed patterns set is a lossless compression of frequent pattern sets, we can first derive the closed patterns set by applying efficient closed pattern mining methods. However, as discussed in Section 7.5, a closed pattern set is not compact enough, and pattern compression needs to be performed. We could use the pattern compression methods introduced in Section 7.5.1 or explore alternative compression methods such as microclustering using the Jaccard coefficient (Chapter 2) and then selecting the most representative patterns from each cluster.

"*How, then, can we assign weights for each context indicator?*" A good weighting function should obey the following properties: (1) the best semantic indicator of a pattern, p, is itself, (2) assign the same score to two patterns if they are equally strong, and (3) if two patterns are independent, neither can indicate the meaning of the other. The meaning of a pattern, p, can be inferred from either the appearance or absence of indicators.

Mutual information is one of several possible weighting functions. It is widely used in information theory to measure the mutual independency of two random variables. Intuitively, it measures how much information a random variable tells about the other. Given two frequent patterns, p_α and p_β, let $X = \{0,1\}$ and $Y = \{0,1\}$ be two random variables representing the appearance of p_α and p_β, respectively. **Mutual information** $I(X;Y)$ is computed as

$$I(X;Y) = \sum_{x \in X} \sum_{y \in Y} P(x,y) log \frac{P(x,y)}{P(x)P(y)}, \tag{7.18}$$

where $P(x=1,y=1)=\frac{|D_\alpha \cap D_\beta|}{|D|}$, $P(x=0,y=1)=\frac{|D_\beta|-|D_\alpha \cap D_\beta|}{|D|}$, $P(x=1,y=0)=\frac{|D_\alpha|-|D_\alpha \cap D_\beta|}{|D|}$, and $P(x=0,y=0)=\frac{|D|-|D_\alpha \cup D_\beta|}{|D|}$. Standard Laplace smoothing can be used to avoid zero probability.

Mutual information favors strongly correlated units and thus can be used to model the indicative strength of the context units selected. With context modeling, pattern annotation can be accomplished as follows:

1. To extract the most significant context indicators, we can use cosine similarity (Chapter 2) to measure the semantic similarity between pairs of context vectors, rank the context indicators by the weight strength, and extract the strongest ones.
2. To extract representative transactions, represent each transaction as a context vector. Rank the transactions with semantic similarity to the pattern p.
3. To extract semantically similar patterns, rank each frequent pattern, p, by the semantic similarity between their context models and the context of p.

Based on these principles, experiments have been conducted on large data sets to generate semantic annotations. Example 7.16 illustrates one such experiment.

Example 7.16 **Semantic annotations generated for frequent patterns from the DBLP Computer Science Bibliography.** Table 7.4 shows annotations generated for frequent patterns from a portion of the DBLP data set.[3] The DBLP data set contains papers from the proceedings of 12 major conferences in the fields of database systems, information retrieval, and data mining. Each transaction consists of two parts: the authors and the title of the corresponding paper.

Consider two types of patterns: (1) *frequent author* or *coauthorship*, each of which is a frequent itemset of authors, and (2) *frequent title terms*, each of which is a frequent sequential pattern of the title words. The method can automatically generate dictionary-like annotations for different kinds of frequent patterns. For frequent itemsets like coauthorship or single authors, the strongest context indicators are usually the other coauthors and discriminative title terms that appear in their work. The semantically similar patterns extracted also reflect the authors and terms related to their work. However, these similar patterns may not even co-occur with the given pattern in a paper. For example, the patterns "*timos_k_selli*," "*ramakrishnan_srikant*," and so on, do not co-occur with the pattern "*christos_faloutsos*," but are extracted because their contexts are similar since they all are database and/or data mining researchers; thus the annotation is meaningful.

For the title term "*information retrieval*," which is a sequential pattern, its strongest context indicators are usually the authors who tend to use the term in the titles of their papers, or the terms that tend to coappear with it. Its semantically similar patterns usually provide interesting concepts or descriptive terms, which are close in meaning (e.g., "*information retrieval* $\rightarrow$ *information filter*)."

[3] *www.informatik.uni-trier.de/~ley/db/*.

Table 7.4 Annotations Generated for Frequent Patterns in the DBLP Data Set

Pattern	***Type***	***Annotations***
christos_faloutsos	Context indicator	spiros_papadimitriou; fast; use fractal; graph; use correlate
	Representative transactions	multi-attribute hash use gray code
	Representative transactions	recovery latent time-series observe sum network tomography particle filter
	Representative transactions	index multimedia database tutorial
	Semantic similar patterns	spiros_papadimitriou&christos_faloutsos; spiros_papadimitriou; flip_korn; timos_k_selli; ramakrishnan_srikant; ramakrishnan_srikant&rakesh_agrawal
information retrieval	Context indicator	w_bruce_croft; web information; monika_ rauch_henzinger; james_p_callan; full-text
	Representative transactions	web information retrieval
	Representative transactions	language model information retrieval
	Semantic similar patterns	information use; web information; probabilistic information; information filter; text information

In both scenarios, the representative transactions extracted give us the titles of papers that effectively capture the meaning of the given patterns. The experiment demonstrates the effectiveness of semantic pattern annotation to generate a dictionary-like annotation for frequent patterns, which can help a user understand the meaning of annotated patterns. ■

The context modeling and semantic analysis method presented here is general and can deal with any type of frequent patterns with context information. Such semantic annotations can have many other applications such as ranking patterns, categorizing and clustering patterns with semantics, and summarizing databases. Applications of the pattern context model and semantical analysis method are also not limited to pattern annotation; other example applications include pattern compression, transaction clustering, pattern relations discovery, and pattern synonym discovery.

7.6.2 Applications of Pattern Mining

We have studied many aspects of frequent pattern mining, with topics ranging from efficient mining algorithms and the diversity of patterns to pattern interestingness, pattern compression/approximation, and semantic pattern annotation. Let's take a moment to consider why this field has generated so much attention. What are some of the application areas in which frequent pattern mining is useful? This section presents an overview of applications for frequent pattern mining. We have touched on several application areas already, such as market basket analysis and correlation analysis, yet frequent pattern mining can be applied to many other areas as well. These range from data preprocessing and classification to clustering and the analysis of complex data.

To summarize, frequent pattern mining is a data mining task that discovers patterns that occur frequently together and/or have some distinctive properties that distinguish them from others, often disclosing something inherent and valuable. The patterns may be itemsets, subsequences, substructures, or values. The task also includes the discovery of rare patterns, revealing items that occur very rarely together yet are of interest. Uncovering frequent patterns and rare patterns leads to many broad and interesting applications, described as follows.

Pattern mining is widely used for **noise filtering and data cleaning** as **preprocessing** in many data-intensive applications. We can use it to analyze microarray data, for instance, which typically consists of tens of thousands of dimensions (e.g., representing genes). Such data can be rather noisy. Frequent pattern data mining can help us distinguish between what is noise and what isn't. We may assume that items that occur frequently together are less likely to be random noise and should not be filtered out. On the other hand, those that occur very frequently (similar to stopwords in text documents) are likely indistinctive and may be filtered out. Frequent pattern mining can help in background information identification and noise reduction.

Pattern mining often helps in the **discovery of inherent structures and clusters hidden in the data**. Given the DBLP data set, for instance, frequent pattern mining can easily find interesting clusters like coauthor clusters (by examining authors who frequently collaborate) and conference clusters (by examining the sharing of many common authors and terms). Such structure or cluster discovery can be used as preprocessing for more sophisticated data mining.

Although there are numerous classification methods (Chapters 8 and 9), research has found that frequent patterns can be used as building blocks in the construction of high-quality classification models, hence called **pattern-based classification**. The approach is successful because (1) the appearance of very infrequent item(s) or itemset(s) can be caused by random noise and may not be reliable for model construction, yet a relatively frequent pattern often carries more information gain for constructing more reliable models; (2) patterns in general (i.e., itemsets consisting of multiple attributes) usually carry more information gain than a single attribute (feature); and (3) the patterns so generated are often intuitively understandable and easy to explain. Recent research has reported several methods that mine interesting, frequent, and discriminative patterns and use them for effective classification. Pattern-based classification methods are introduced in Chapter 9.

Frequent patterns can also be used effectively for **subspace clustering in high-dimensional space**. Clustering is challenging in high-dimensional space, where the distance between two objects is often difficult to measure. This is because such a distance is dominated by the different sets of dimensions in which the objects are residing.

Thus, instead of clustering objects in their full high-dimensional spaces, it can be more meaningful to find clusters in certain subspaces. Recently, researchers have developed subspace-based pattern growth methods that cluster objects based on their common frequent patterns. They have shown that such methods are effective for clustering microarray-based gene expression data. Subspace clustering methods are discussed in Chapter 11.

Pattern analysis is useful in the **analysis of spatiotemporal data, time-series data, image data, video data, and multimedia data**. An area of *spatiotemporal data analysis* is the discovery of **colocation patterns**. These, for example, can help determine if a certain disease is geographically colocated with certain objects like a well, a hospital, or a river. In *time-series data analysis*, researchers have discretized time-series values into multiple intervals (or levels) so that tiny fluctuations and value differences can be ignored. The data can then be summarized into sequential patterns, which can be indexed to facilitate similarity search or comparative analysis. In *image analysis and pattern recognition*, researchers have also identified frequently occurring visual fragments as "visual words," which can be used for effective clustering, classification, and comparative analysis.

Pattern mining has also been used for the **analysis of sequence or structural data** such as trees, graphs, subsequences, and networks. In software engineering, researchers have identified consecutive or gapped subsequences in program execution as sequential patterns that help identify software bugs. Copy-and-paste bugs in large software programs can be identified by extended sequential pattern analysis of source programs. Plagiarized software programs can be identified based on their essentially identical program flow/loop structures. Authors' commonly used sentence substructures can be identified and used to distinguish articles written by different authors.

Frequent and discriminative patterns can be used as primitive **indexing structures** (known as graph indices) to help search large, complex, structured data sets and networks. These support a similarity search in graph-structured data such as chemical compound databases or XML-structured databases. Such patterns can also be used for data compression and summarization.

Furthermore, frequent patterns have been used in **recommender systems**, where people can find correlations, clusters of customer behaviors, and classification models based on commonly occurring or discriminative patterns (Chapter 13).

Finally, studies on efficient computation methods in pattern mining mutually enhance many other studies on **scalable computation**. For example, the computation and materialization of **iceberg cubes** using the BUC and Star-Cubing algorithms (Chapter 5) respectively share many similarities to computing frequent patterns by the Apriori and FP-growth algorithms (Chapter 6).

7.7 Summary

- The **scope** of frequent pattern mining research reaches far beyond the basic concepts and methods introduced in Chapter 6 for mining frequent itemsets and associations. This chapter presented a road map of the field, where topics are organized with respect to the kinds of patterns and rules that can be mined, mining methods, and applications.

- In addition to mining for basic frequent itemsets and associations, **advanced forms of patterns** can be mined such as multilevel associations and multidimensional associations, quantitative association rules, rare patterns, and negative patterns. We can also mine high-dimensional patterns and compressed or approximate patterns.
- **Multilevel associations** involve data at more than one abstraction level (e.g., "*buys computer*" and "*buys laptop*"). These may be mined using multiple minimum support thresholds. **Multidimensional associations** contain more than one dimension. Techniques for mining such associations differ in how they handle repetitive predicates. **Quantitative association rules** involve quantitative attributes. Discretization, clustering, and statistical analysis that discloses exceptional behavior can be integrated with the pattern mining process.
- **Rare patterns** occur rarely but are of special interest. **Negative patterns** are patterns with components that exhibit negatively correlated behavior. Care should be taken in the definition of negative patterns, with consideration of the null-invariance property. Rare and negative patterns may highlight exceptional behavior in the data, which is likely of interest.
- **Constraint-based mining** strategies can be used to help direct the mining process toward patterns that match users' intuition or satisfy certain constraints. Many user-specified constraints can be pushed deep into the mining process. Constraints can be categorized into **pattern-pruning** and **data-pruning** constraints. Properties of such constraints include *monotonicity*, *antimonotonicity*, *data-antimonotonicity*, and *succinctness*. Constraints with such properties can be properly incorporated into efficient pattern mining processes.
- Methods have been developed for mining patterns in **high-dimensional space**. This includes a pattern growth approach based on *row enumeration* for mining data sets where the number of dimensions is large and the number of data tuples is small (e.g., for microarray data), as well as mining **colossal patterns** (i.e., patterns of very long length) by a *Pattern-Fusion* method.
- To reduce the number of patterns returned in mining, we can instead mine compressed patterns or approximate patterns. *Compressed patterns* can be mined with representative patterns defined based on the concept of clustering, and *approximate patterns* can be mined by extracting **redundancy-aware top-*k* patterns** (i.e., a small set of k-representative patterns that have not only high significance but also low redundancy with respect to one another).
- **Semantic annotations** can be generated to help users understand the meaning of the frequent patterns found, such as for textual terms like "{*frequent, pattern*}." These are dictionary-like annotations, providing semantic information relating to the term. This information consists of *context indicators* (e.g., terms indicating the context of that pattern), the most *representative data transactions* (e.g., fragments or sentences

containing the term), and the most *semantically similar patterns* (e.g., "{*maximal, pattern*}" is semantically similar to "{*frequent, pattern*}"). The annotations provide a view of the pattern's context from different angles, which aids in their understanding.

- Frequent pattern mining has many diverse applications, ranging from pattern-based data cleaning to pattern-based classification, clustering, and outlier or exception analysis. These methods are discussed in the subsequent chapters in this book.

7.8 Exercises

7.1 Propose and outline a **level-shared mining** approach to mining multilevel association rules in which each item is encoded by its level position. Design it so that an initial scan of the database collects the count for each item *at each concept level*, identifying frequent and subfrequent items. Comment on the processing cost of mining multilevel associations with this method in comparison to mining single-level associations.

7.2 Suppose, as manager of a chain of stores, you would like to use sales transactional data to analyze the effectiveness of your store's advertisements. In particular, you would like to study how specific factors influence the effectiveness of advertisements that announce a particular category of items on sale. The factors to study are the *region* in which customers live and the *day-of-the-week* and *time-of-the-day* of the ads. Discuss how to design an efficient method to mine the transaction data sets and explain how **multidimensional** and **multilevel mining** methods can help you derive a good solution.

7.3 **Quantitative association rules** may disclose exceptional behaviors within a data set, where "exceptional" can be defined based on statistical theory. For example, Section 7.2.3 shows the association rule

$$sex = female \Rightarrow mean\_wage = \$7.90/hr\ (overall\_mean\_wage = \$9.02/hr),$$

which suggests an exceptional pattern. The rule states that the average wage for females is only $7.90 per hour, which is a significantly lower wage than the overall average of $9.02 per hour. Discuss how such quantitative rules can be discovered systematically and efficiently in large data sets with quantitative attributes.

7.4 In multidimensional data analysis, it is interesting to extract pairs of *similar* cell characteristics associated with substantial changes in measure in a data cube, where cells are considered *similar* if they are related by roll-up (i.e, *ancestors*), drill-down (i.e, *descendants*), or 1-D mutation (i.e, *siblings*) operations. Such an analysis is called **cube gradient analysis**.

Suppose the measure of the cube is *average*. A user poses a set of *probe cells* and would like to find their corresponding sets of *gradient cells*, each of which satisfies a certain gradient threshold. For example, find the set of corresponding gradient cells that have an average sale price greater than 20% of that of the given probe cells. Develop an algorithm than mines the set of constrained gradient cells efficiently in a large data cube.

7.5 Section 7.2.4 presented various ways of defining negatively correlated patterns. Consider Definition 7.3: "Suppose that itemsets X and Y are both frequent, that is, $sup(X) \geq min\_sup$ and $sup(Y) \geq min\_sup$, where min_sup is the minimum support threshold. If $(P(X|Y) + P(Y|X))/2 < \epsilon$, where ϵ is a negative pattern threshold, then pattern $X \cup Y$ is a **negatively correlated pattern**." Design an efficient pattern growth algorithm for mining the set of negatively correlated patterns.

7.6 Prove that each entry in the following table correctly characterizes its corresponding **rule constraint** for frequent itemset mining.

	Rule Constraint	*Antimonotonic*	*Monotonic*	*Succinct*
(a)	$v \in S$	no	yes	yes
(b)	$S \subseteq V$	yes	no	yes
(c)	$min(S) \leq v$	no	yes	yes
(d)	$range(S) \leq v$	yes	no	no
(e)	$variance(S) \leq v$	convertible	convertible	no

7.7 The price of each item in a store is non-negative. The store manager is only interested in rules of certain forms, using the constraints given in (a)–(b). For each of the following cases, identify the kinds of **constraints** they represent and briefly discuss how to mine such association rules using **constraint-based pattern mining**.

(a) Containing at least one Blu-ray DVD movie.

(b) Containing items with a sum of the prices that is less than \$150.

(c) Containing one free item and other items with a sum of the prices that is at least \$200.

(d) Where the average price of all the items is between \$100 and \$500.

7.8 Section 7.4.1 introduced a core Pattern-Fusion method for **mining high-dimensional data**. Explain why a long pattern, if one exists in the data set, is likely to be discovered by this method.

7.9 Section 7.5.1 defined a **pattern distance measure** between closed patterns P_1 and P_2 as

$$Pat\_Dist(P_1, P_2) = 1 - \frac{|T(P_1) \cap T(P_2)|}{|T(P_1) \cup T(P_2)|},$$

where $T(P_1)$ and $T(P_2)$ are the supporting transaction sets of P_1 and P_2, respectively. Is this a valid distance metric? Show the derivation to support your answer.

7.10 Association rule mining often generates a large number of rules, many of which may be similar, thus not containing much novel information. Design an efficient algorithm that **compresses** a large set of patterns into a small compact set. Discuss whether your mining method is robust under different pattern similarity definitions.

7.11 Frequent pattern mining may generate many superfluous patterns. Therefore, it is important to develop methods that mine compressed patterns. Suppose a user would like to obtain only k patterns (where k is a small integer). Outline an efficient method that generates the ***k* most representative patterns**, where more distinct patterns are preferred over very similar patterns. Illustrate the effectiveness of your method using a small data set.

7.12 It is interesting to generate **semantic annotations** for mined patterns. Section 7.6.1 presented a pattern annotation method. Alternative methods are possible, such as by utilizing type information. In the DBLP data set, for example, authors, conferences, terms, and papers form multi-typed data. Develop a method for automated semantic pattern annotation that makes good use of typed information.

7.9 Bibliographic Notes

This chapter described various ways in which the basic techniques of frequent itemset mining (presented in Chapter 6) have been extended. One line of extension is mining multilevel and multidimensional association rules. Multilevel association mining was studied in Srikant and Agrawal [SA95] and Han and Fu [HF95]. In Srikant and Agrawal [SA95], such mining was studied in the context of *generalized association rules*, and an R-interest measure was proposed for removing redundant rules. Mining multidimensional association rules using static discretization of quantitative attributes and data cubes was studied by Kamber, Han, and Chiang [KHC97].

Another line of extension is to mine patterns on numeric attributes. Srikant and Agrawal [SA96] proposed a nongrid-based technique for mining quantitative association rules, which uses a measure of partial completeness. Mining quantitative association rules based on rule clustering was proposed by Lent, Swami, and Widom [LSW97]. Techniques for mining quantitative rules based on x-monotone and rectilinear regions were presented by Fukuda, Morimoto, Morishita, and Tokuyama [FMMT96] and Yoda, Fukuda, Morimoto, et al. [YFM$^+$97]. Mining (distance-based) association rules over interval data was proposed by Miller and Yang [MY97]. Aumann and Lindell [AL99] studied the mining of quantitative association rules based on a statistical theory to present only those rules that deviate substantially from normal data.

Mining rare patterns by pushing group-based constraints was proposed by Wang, He, and Han [WHH00]. Mining negative association rules was discussed by Savasere, Omiecinski, and Navathe [SON98] and by Tan, Steinbach, and Kumar [TSK05].

Constraint-based mining directs the mining process toward patterns that are likely of interest to the user. The use of metarules as syntactic or semantic filters defining the form of interesting single-dimensional association rules was proposed in Klemettinen, Mannila, Ronkainen, et al. [KMR$^+$94]. Metarule-guided mining, where the metarule consequent specifies an action (e.g., Bayesian clustering or plotting) to be applied to the data satisfying the metarule antecedent, was proposed in Shen, Ong, Mitbander, and Zaniolo [SOMZ96]. A relation-based approach to metarule-guided mining of association rules was studied in Fu and Han [FH95].

Methods for constraint-based mining using pattern pruning constraints were studied by Ng, Lakshmanan, Han, and Pang [NLHP98]; Lakshmanan, Ng, Han, and Pang [LNHP99]; and Pei, Han, and Lakshmanan [PHL01]. Constraint-based pattern mining by data reduction using data pruning constraints was studied by Bonchi, Giannotti, Mazzanti, and Pedreschi [BGMP03] and Zhu, Yan, Han, and Yu [ZYHY07]. An efficient method for mining constrained correlated sets was given in Grahne, Lakshmanan, and Wang [GLW00]. A dual mining approach was proposed by Bucila, Gehrke, Kifer, and White [BGKW03]. Other ideas involving the use of templates or predicate constraints in mining have been discussed in Anand and Kahn [AK93]; Dhar and Tuzhilin [DT93]; Hoschka and Klösgen [HK91]; Liu, Hsu, and Chen [LHC97]; Silberschatz and Tuzhilin [ST96]; and Srikant, Vu, and Agrawal [SVA97].

Traditional pattern mining methods encounter challenges when mining high-dimensional patterns, with applications like bioinformatics. Pan, Cong, Tung, et al. [PCT$^+$03] proposed CARPENTER, a method for finding closed patterns in high-dimensional biological data sets, which integrates the advantages of vertical data formats and pattern growth methods. Pan, Tung, Cong, and Xu [PTCX04] proposed COBBLER, which finds frequent closed itemsets by integrating row enumeration with column enumeration. Liu, Han, Xin, and Shao [LHXS06] proposed TDClose to mine frequent closed patterns in high-dimensional data by starting from the maximal rowset, integrated with a row-enumeration tree. It uses the pruning power of the minimum support threshold to reduce the search space. For mining rather long patterns, called *colossal patterns*, Zhu, Yan, Han, et al. [ZYH$^+$07] developed a core Pattern-Fusion method that leaps over an exponential number of intermediate patterns to reach colossal patterns.

To generate a reduced set of patterns, recent studies have focused on mining compressed sets of frequent patterns. Closed patterns can be viewed as a lossless compression of frequent patterns, whereas maximal patterns can be viewed as a simple lossy compression of frequent patterns. Top-k patterns, such as by Wang, Han, Lu, and Tsvetkov [WHLT05], and error-tolerant patterns, such as by Yang, Fayyad, and Bradley [YFB01], are alternative forms of interesting patterns. Afrati, Gionis, and Mannila [AGM04] proposed to use k-itemsets to cover a collection of frequent itemsets. For frequent itemset compression, Yan, Cheng, Han, and Xin [YCHX05] proposed a profile-based approach, and Xin, Han, Yan, and Cheng [XHYC05] proposed a clustering-based approach. By taking into consideration both pattern significance and pattern redundancy, Xin, Cheng, Yan, and Han [XCYH06] proposed a method for extracting redundancy-aware top-k patterns.

Automated semantic annotation of frequent patterns is useful for explaining the meaning of patterns. Mei, Xin, Cheng, et al. [MXC$^+$07] studied methods for semantic annotation of frequent patterns.

An important extension to frequent itemset mining is mining sequence and structural data. This includes mining sequential patterns (Agrawal and Srikant [AS95]; Pei, Han, Mortazavi-Asl, et al. [PHM-A$^+$01, PHM-A$^+$04]; and Zaki [Zak01]); mining frequent espisodes (Mannila, Toivonen, and Verkamo [MTV97]); mining structural patterns (Inokuchi, Washio, and Motoda [IWM98]; Kuramochi and Karypis [KK01]; and Yan and Han [YH02]); mining cyclic association rules (Özden, Ramaswamy, and Silberschatz [ORS98]); intertransaction association rule mining (Lu, Han, and Feng [LHF98]); and calendric market basket analysis (Ramaswamy, Mahajan, and Silberschatz [RMS98]). Mining such patterns is considered an advanced topic and readers are referred to these sources.

Pattern mining has been extended to help effective data classification and clustering. Pattern-based classification (Liu, Hsu, and Ma [LHM98] and Cheng, Yan, Han, and Hsu [CYHH07]) is discussed in Chapter 9. Pattern-based cluster analysis (Agrawal, Gehrke, Gunopulos, and Raghavan [AGGR98] and H. Wang, W. Wang, Yang, and Yu [WWYY02]) is discussed in Chapter 11.

Pattern mining also helps many other data analysis and processing tasks such as cube gradient mining and discriminative analysis (Imielinski, Khachiyan, and Abdulghani [IKA02]; Dong, Han, Lam, et al. [DHL$^+$04]; Ji, Bailey, and Dong [JBD05]), discriminative pattern-based indexing (Yan, Yu, and Han [YYH05]), and discriminative pattern-based similarity search (Yan, Zhu, Yu, and Han [YZYH06]).

Pattern mining has been extended to mining spatial, temporal, time-series, and multimedia data, and data streams. Mining spatial association rules or spatial collocation rules was studied by Koperski and Han [KH95]; Xiong, Shekhar, Huang, et al. [XSH$^+$04]; and Cao, Mamoulis, and Cheung [CMC05]. Pattern-based mining of time-series data is discussed in Shieh and Keogh [SK08] and Ye and Keogh [YK09]. There are many studies on pattern-based mining of multimedia data such as Zaïane, Han, and Zhu [ZHZ00] and Yuan, Wu, and Yang [YWY07]. Methods for mining frequent patterns on stream data have been proposed by many researchers, including Manku and Motwani [MM02]; Karp, Papadimitriou, and Shenker [KPS03]; and Metwally, Agrawal, and El Abbadi [MAE05]. These pattern mining methods are considered advanced topics.

Pattern mining has broad applications. Application areas include computer science such as software bug analysis, sensor network mining, and performance improvement of operating systems. For example, CP-Miner by Li, Lu, Myagmar, and Zhou [LLMZ04] uses pattern mining to identify copy-pasted code for bug isolation. PR-Miner by Li and Zhou [LZ05] uses pattern mining to extract application-specific programming rules from source code. Discriminative pattern mining is used for program failure detection to classify software behaviors (Lo, Cheng, Han, et al. [LCH$^+$09]) and for troubleshooting in sensor networks (Khan, Le, Ahmadi, et al. [KLA$^+$08]).

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8 Classification: Basic Concepts

Classification is a form of data analysis that extracts models describing important data classes. Such models, called classifiers, predict categorical (discrete, unordered) class labels. For example, we can build a classification model to categorize bank loan applications as either safe or risky. Such analysis can help provide us with a better understanding of the data at large. Many classification methods have been proposed by researchers in machine learning, pattern recognition, and statistics. Most algorithms are memory resident, typically assuming a small data size. Recent data mining research has built on such work, developing scalable classification and prediction techniques capable of handling large amounts of disk-resident data. Classification has numerous applications, including fraud detection, target marketing, performance prediction, manufacturing, and medical diagnosis.

We start off by introducing the main ideas of classification in Section 8.1. In the rest of this chapter, you will learn the basic techniques for data classification such as how to build decision tree classifiers (Section 8.2), Bayesian classifiers (Section 8.3), and rule-based classifiers (Section 8.4). Section 8.5 discusses how to evaluate and compare different classifiers. Various measures of accuracy are given as well as techniques for obtaining reliable accuracy estimates. Methods for increasing classifier accuracy are presented in Section 8.6, including cases for when the data set is class imbalanced (i.e., where the main class of interest is rare).

8.1 Basic Concepts

We introduce the concept of classification in Section 8.1.1. Section 8.1.2 describes the general approach to classification as a two-step process. In the first step, we build a classification model based on previous data. In the second step, we determine if the model's accuracy is acceptable, and if so, we use the model to classify new data.

8.1.1 What Is Classification?

A bank loans officer needs analysis of her data to learn which loan applicants are "safe" and which are "risky" for the bank. A marketing manager at *AllElectronics* needs data analysis to help guess whether a customer with a given profile will buy a new computer. A medical researcher wants to analyze breast cancer data to predict which one of three specific treatments a patient should receive. In each of these examples, the data analysis task is **classification**, where a model or **classifier** is constructed to predict *class (categorical) labels*, such as "safe" or "risky" for the loan application data; "yes" or "no" for the marketing data; or "treatment A," "treatment B," or "treatment C" for the medical data. These categories can be represented by discrete values, where the ordering among values has no meaning. For example, the values 1, 2, and 3 may be used to represent treatments A, B, and C, where there is no ordering implied among this group of treatment regimes.

Suppose that the marketing manager wants to predict how much a given customer will spend during a sale at *AllElectronics*. This data analysis task is an example of **numeric prediction**, where the model constructed predicts a *continuous-valued function*, or *ordered value*, as opposed to a class label. This model is a **predictor**. **Regression analysis** is a statistical methodology that is most often used for numeric prediction; hence the two terms tend to be used synonymously, although other methods for numeric prediction exist. Classification and numeric prediction are the two major types of **prediction problems**. This chapter focuses on classification.

8.1.2 General Approach to Classification

"How does classification work?" **Data classification** is a two-step process, consisting of a *learning step* (where a classification model is constructed) and a *classification step* (where the model is used to predict class labels for given data). The process is shown for the loan application data of Figure 8.1. (The data are simplified for illustrative purposes. In reality, we may expect many more attributes to be considered.

In the first step, a classifier is built describing a predetermined set of data classes or concepts. This is the **learning step** (or training phase), where a classification algorithm builds the classifier by analyzing or "learning from" a **training set** made up of database tuples and their associated class labels. A tuple, $\boldsymbol{X}$, is represented by an n-dimensional **attribute vector**, $\boldsymbol{X} = (x_1, x_2, \ldots, x_n)$, depicting n measurements made on the tuple from n database attributes, respectively, $A_1, A_2, \ldots, A_n$.[1] Each tuple, $\boldsymbol{X}$, is assumed to belong to a predefined class as determined by another database attribute called the **class label attribute**. The class label attribute is discrete-valued and unordered. It is *categorical* (or nominal) in that each value serves as a category or class. The individual tuples making up the training set are referred to as **training tuples** and are randomly sampled from the database under analysis. In the context of classification, data tuples can be referred to as *samples, examples, instances, data points*, or *objects*.[2]

[1]Each attribute represents a "feature" of $\boldsymbol{X}$. Hence, the pattern recognition literature uses the term *feature vector* rather than *attribute vector*. In our discussion, we use the term attribute vector, and in our notation, any variable representing a vector is shown in bold italic font; measurements depicting the vector are shown in italic font (e.g., $\boldsymbol{X} = (x_1, x_2, x_3)$).

[2]In the machine learning literature, training tuples are commonly referred to as *training samples*. Throughout this text, we prefer to use the term *tuples* instead of *samples*.

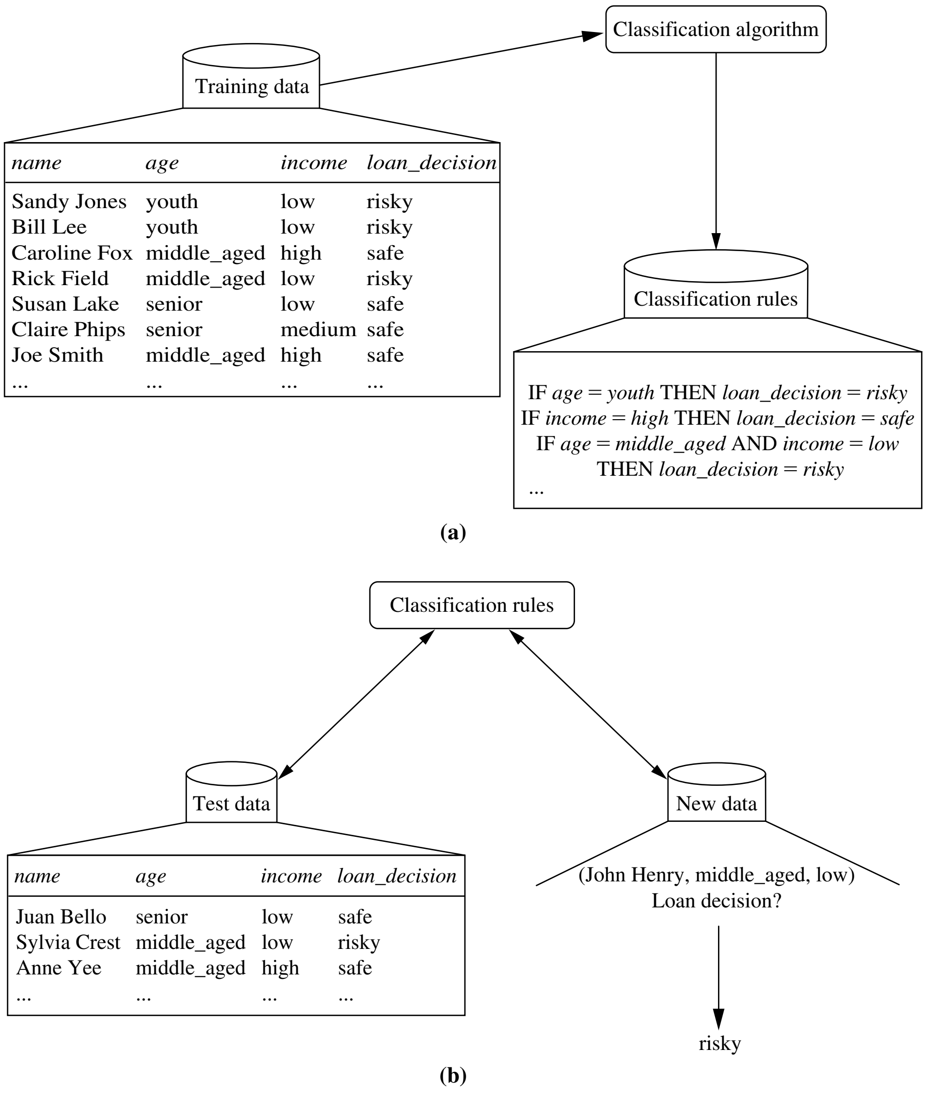

Training data
Classification algorithm
Classification rules
name | age | income | loan_decision
Sandy Jones youth low risky
Bill Lee youth low risky
Caroline Fox middle_aged high safe
Rick Field middle_aged low risky
Susan Lake senior low safe
Claire Phips senior medium safe
Joe Smith middle_aged high safe
IF *age* = *youth* THEN *loan_decision* = *risky*
IF *income* = *high* THEN *loan_decision* = *safe*
IF *age* = *middle_aged* AND *income* = *low* THEN *loan_decision* = *risky*
(a)
Classification rules
Test data
New data
name | age | income | loan_decision
Juan Bello senior low safe
Sylvia Crest middle_aged low risky
Anne Yee middle_aged high safe
(John Henry, middle_aged, low)
Loan decision?
risky
(b)

Figure 8.1 The data classification process: (a) *Learning*: Training data are analyzed by a classification algorithm. Here, the class label attribute is *loan_decision*, and the learned model or classifier is represented in the form of classification rules. (b) *Classification*: Test data are used to estimate the accuracy of the classification rules. If the accuracy is considered acceptable, the rules can be applied to the classification of new data tuples.

Because the class label of each training tuple *is provided*, this step is also known as **supervised learning** (i.e., the learning of the classifier is "supervised" in that it is told to which class each training tuple belongs). It contrasts with **unsupervised learning** (or **clustering**), in which the class label of each training tuple is not known, and the number or set of classes to be learned may not be known in advance. For example, if we did not have the *loan_decision* data available for the training set, we could use clustering to try to determine "groups of like tuples," which may correspond to risk groups within the loan application data. Clustering is the topic of Chapters 10 and 11.

This first step of the classification process can also be viewed as the learning of a mapping or function, $y = f(\boldsymbol{X})$, that can predict the associated class label y of a given tuple $\boldsymbol{X}$. In this view, we wish to learn a mapping or function that separates the data classes. Typically, this mapping is represented in the form of classification rules, decision trees, or mathematical formulae. In our example, the mapping is represented as classification rules that identify loan applications as being either safe or risky (Figure 8.1a). The rules can be used to categorize future data tuples, as well as provide deeper insight into the data contents. They also provide a compressed data representation.

"*What about classification accuracy?*" In the second step (Figure 8.1b), the model is used for classification. First, the predictive accuracy of the classifier is estimated. If we were to use the training set to measure the classifier's accuracy, this estimate would likely be optimistic, because the classifier tends to **overfit** the data (i.e., during learning it may incorporate some particular anomalies of the training data that are not present in the general data set overall). Therefore, a **test set** is used, made up of **test tuples** and their associated class labels. They are independent of the training tuples, meaning that they were not used to construct the classifier.

The **accuracy** of a classifier on a given test set is the percentage of test set tuples that are correctly classified by the classifier. The associated class label of each test tuple is compared with the learned classifier's class prediction for that tuple. Section 8.5 describes several methods for estimating classifier accuracy. If the accuracy of the classifier is considered acceptable, the classifier can be used to classify future data tuples for which the class label is not known. (Such data are also referred to in the machine learning literature as "unknown" or "previously unseen" data.) For example, the classification rules learned in Figure 8.1(a) from the analysis of data from previous loan applications can be used to approve or reject new or future loan applicants.

8.2 Decision Tree Induction

Decision tree induction is the learning of decision trees from class-labeled training tuples. A **decision tree** is a flowchart-like tree structure, where each **internal node** (nonleaf node) denotes a test on an attribute, each **branch** represents an outcome of the test, and each **leaf node** (or *terminal node*) holds a class label. The topmost node in a tree is the **root** node. A typical decision tree is shown in Figure 8.2. It represents the concept *buys_computer*, that is, it predicts whether a customer at *AllElectronics* is

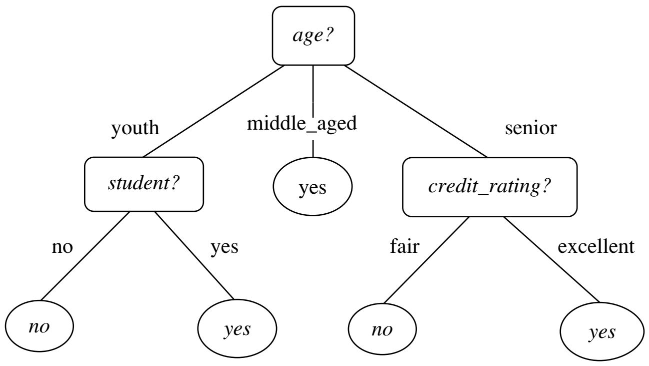


Figure 8.2 A decision tree for the concept *buys_computer*, indicating whether an *AllElectronics* customer is likely to purchase a computer. Each internal (nonleaf) node represents a test on an attribute. Each leaf node represents a class (either *buys_computer* = *yes* or *buys_computer* = *no*).

likely to purchase a computer. Internal nodes are denoted by rectangles, and leaf nodes are denoted by ovals. Some decision tree algorithms produce only *binary* trees (where each internal node branches to exactly two other nodes), whereas others can produce nonbinary trees.

"*How are decision trees used for classification?*" Given a tuple, $\boldsymbol{X}$, for which the associated class label is unknown, the attribute values of the tuple are tested against the decision tree. A path is traced from the root to a leaf node, which holds the class prediction for that tuple. Decision trees can easily be converted to classification rules.

"*Why are decision tree classifiers so popular?*" The construction of decision tree classifiers does not require any domain knowledge or parameter setting, and therefore is appropriate for exploratory knowledge discovery. Decision trees can handle multidimensional data. Their representation of acquired knowledge in tree form is intuitive and generally easy to assimilate by humans. The learning and classification steps of decision tree induction are simple and fast. In general, decision tree classifiers have good accuracy. However, successful use may depend on the data at hand. Decision tree induction algorithms have been used for classification in many application areas such as medicine, manufacturing and production, financial analysis, astronomy, and molecular biology. Decision trees are the basis of several commercial rule induction systems.

In Section 8.2.1, we describe a basic algorithm for learning decision trees. During tree construction, *attribute selection measures* are used to select the attribute that best partitions the tuples into distinct classes. Popular measures of attribute selection are given in Section 8.2.2. When decision trees are built, many of the branches may reflect noise or outliers in the training data. *Tree pruning* attempts to identify and remove such branches, with the goal of improving classification accuracy on unseen data. Tree pruning is described in Section 8.2.3. Scalability issues for the induction of decision trees from large databases are discussed in Section 8.2.4. Section 8.2.5 presents a visual mining approach to decision tree induction.

8.2.1 Decision Tree Induction

During the late 1970s and early 1980s, J. Ross Quinlan, a researcher in machine learning, developed a decision tree algorithm known as **ID3** (Iterative Dichotomiser). This work expanded on earlier work on *concept learning systems*, described by E. B. Hunt, J. Marin, and P. T. Stone. Quinlan later presented **C4.5** (a successor of ID3), which became a benchmark to which newer supervised learning algorithms are often compared. In 1984, a group of statisticians (L. Breiman, J. Friedman, R. Olshen, and C. Stone) published the book *Classification and Regression Trees* (**CART**), which described the generation of binary decision trees. ID3 and CART were invented independently of one another at around the same time, yet follow a similar approach for learning decision trees from training tuples. These two cornerstone algorithms spawned a flurry of work on decision tree induction.

ID3, C4.5, and CART adopt a greedy (i.e., nonbacktracking) approach in which decision trees are constructed in a top-down recursive divide-and-conquer manner. Most algorithms for decision tree induction also follow a top-down approach, which starts with a training set of tuples and their associated class labels. The training set is recursively partitioned into smaller subsets as the tree is being built. A basic decision tree algorithm is summarized in Figure 8.3. At first glance, the algorithm may appear long, but fear not! It is quite straightforward. The strategy is as follows.

- The algorithm is called with three parameters: D, *attribute_list*, and *Attribute_selection_method*. We refer to D as a data partition. Initially, it is the complete set of training tuples and their associated class labels. The parameter *attribute_list* is a list of attributes describing the tuples. *Attribute_selection_method* specifies a heuristic procedure for selecting the attribute that "best" discriminates the given tuples according to class. This procedure employs an attribute selection measure such as information gain or the Gini index. Whether the tree is strictly binary is generally driven by the attribute selection measure. Some attribute selection measures, such as the Gini index, enforce the resulting tree to be binary. Others, like information gain, do not, therein allowing multiway splits (i.e., two or more branches to be grown from a node).
- The tree starts as a single node, N, representing the training tuples in D (step 1).[3]

[3]The partition of class-labeled training tuples at node N is the set of tuples that follow a path from the root of the tree to node N when being processed by the tree. This set is sometimes referred to in the literature as the *family* of tuples at node N. We have referred to this set as the "tuples represented at node N," "the tuples that reach node N," or simply "the tuples at node N." Rather than storing the actual tuples at a node, most implementations store pointers to these tuples.

Algorithm: Generate_decision_tree. Generate a decision tree from the training tuples of data partition, *D*.

Input:

- Data partition, *D*, which is a set of training tuples and their associated class labels;
- *attribute_list*, the set of candidate attributes;
- *Attribute_selection_method*, a procedure to determine the splitting criterion that "best" partitions the data tuples into individual classes. This criterion consists of a *splitting_attribute* and, possibly, either a *split-point* or *splitting subset.*

Output: A decision tree.

Method:

```
(1)  create a node $N$;
(2)  if tuples in $D$ are all of the same class, $C$, then
(3)       return $N$ as a leaf node labeled with the class $C$;
(4)  if attribute_list is empty then
(5)       return $N$ as a leaf node labeled with the majority class in $D$; // majority voting
(6)  apply Attribute_selection_method($D$, attribute_list) to find the "best" splitting_criterion;
(7)  label node $N$ with splitting_criterion;
(8)  if splitting_attribute is discrete-valued and
          multiway splits allowed then // not restricted to binary trees
(9)       attribute_list $\leftarrow$ attribute_list $-$ splitting_attribute; // remove splitting_attribute
(10) for each outcome $j$ of splitting_criterion
     // partition the tuples and grow subtrees for each partition
(11)      let $D_j$ be the set of data tuples in $D$ satisfying outcome $j$; // a partition
(12)      if $D_j$ is empty then
(13)           attach a leaf labeled with the majority class in $D$ to node $N$;
(14)      else attach the node returned by Generate_decision_tree($D_j$, attribute_list) to node $N$;
     endfor
(15) return $N$;
```

Figure 8.3 Basic algorithm for inducing a decision tree from training tuples.

- If the tuples in *D* are all of the same class, then node *N* becomes a leaf and is labeled with that class (steps 2 and 3). Note that steps 4 and 5 are terminating conditions. All terminating conditions are explained at the end of the algorithm.
- Otherwise, the algorithm calls *Attribute_selection_method* to determine the **splitting criterion**. The splitting criterion tells us which attribute to test at node *N* by determining the "best" way to separate or partition the tuples in *D* into individual classes (step 6). The splitting criterion also tells us which branches to grow from node *N* with respect to the outcomes of the chosen test. More specifically, the splitting criterion indicates the **splitting attribute** and may also indicate either a **split-point** or a **splitting subset**. The splitting criterion is determined so that, ideally, the resulting

partitions at each branch are as "pure" as possible. A partition is **pure** if all the tuples in it belong to the same class. In other words, if we split up the tuples in D according to the mutually exclusive outcomes of the splitting criterion, we hope for the resulting partitions to be as pure as possible.

- The node N is labeled with the splitting criterion, which serves as a test at the node (step 7). A branch is grown from node N for each of the outcomes of the splitting criterion. The tuples in D are partitioned accordingly (steps 10 to 11). There are three possible scenarios, as illustrated in Figure 8.4. Let A be the splitting attribute. A has v distinct values, $\{a_1, a_2, \ldots, a_v\}$, based on the training data.

1. *A is discrete-valued:* In this case, the outcomes of the test at node N correspond directly to the known values of A. A branch is created for each known value, a_j, of A and labeled with that value (Figure 8.4a). Partition D_j is the subset of class-labeled tuples in D having value a_j of A. Because all the tuples in a

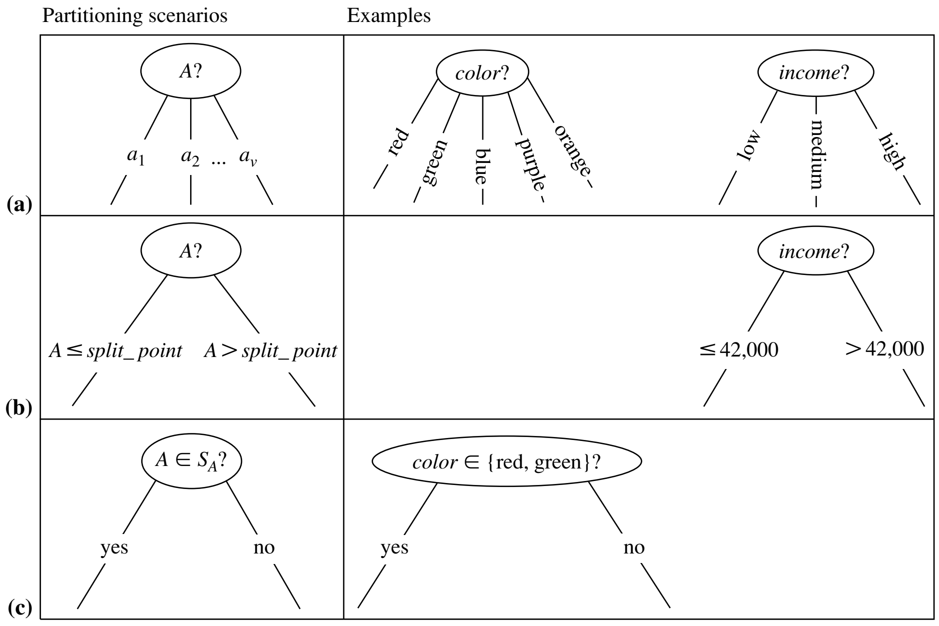


Figure 8.4 This figure shows three possibilities for partitioning tuples based on the splitting criterion, each with examples. Let A be the splitting attribute. (a) If A is discrete-valued, then one branch is grown for each known value of A. (b) If A is continuous-valued, then two branches are grown, corresponding to $A \leq$ *split_point* and $A >$ *split_point*. (c) If A is discrete-valued and a binary tree must be produced, then the test is of the form $A \in S_A$, where S_A is the splitting subset for A.

given partition have the same value for A, A need not be considered in any future partitioning of the tuples. Therefore, it is removed from *attribute_list* (steps 8 and 9).

2. *A is continuous-valued:* In this case, the test at node N has two possible outcomes, corresponding to the conditions $A \leq split\_point$ and $A > split\_point$, respectively, where *split_point* is the split-point returned by *Attribute_selection_method* as part of the splitting criterion. (In practice, the split-point, a, is often taken as the midpoint of two known adjacent values of A and therefore may not actually be a preexisting value of A from the training data.) Two branches are grown from N and labeled according to the previous outcomes (Figure 8.4b). The tuples are partitioned such that D_1 holds the subset of class-labeled tuples in D for which $A \leq split\_point$, while D_2 holds the rest.
3. *A is discrete-valued* and a *binary tree* must be produced (as dictated by the attribute selection measure or algorithm being used): The test at node N is of the form "$A \in S_A$?," where S_A is the splitting subset for A, returned by *Attribute_selection_method* as part of the splitting criterion. It is a subset of the known values of A. If a given tuple has value a_j of A and if $a_j \in S_A$, then the test at node N is satisfied. Two branches are grown from N (Figure 8.4c). By convention, the left branch out of N is labeled *yes* so that D_1 corresponds to the subset of class-labeled tuples in D that satisfy the test. The right branch out of N is labeled *no* so that D_2 corresponds to the subset of class-labeled tuples from D that do not satisfy the test.

- The algorithm uses the same process recursively to form a decision tree for the tuples at each resulting partition, D_j, of D (step 14).
- The recursive partitioning stops only when any one of the following terminating conditions is true:
  1. All the tuples in partition D (represented at node N) belong to the same class (steps 2 and 3).
  2. There are no remaining attributes on which the tuples may be further partitioned (step 4). In this case, **majority voting** is employed (step 5). This involves converting node N into a leaf and labeling it with the most common class in D. Alternatively, the class distribution of the node tuples may be stored.
  3. There are no tuples for a given branch, that is, a partition D_j is empty (step 12). In this case, a leaf is created with the majority class in D (step 13).
- The resulting decision tree is returned (step 15).

The computational complexity of the algorithm given training set D is $O(n \times |D| \times log(|D|))$, where n is the number of attributes describing the tuples in D and $|D|$ is the number of training tuples in D. This means that the computational cost of growing a tree grows at most $n \times |D| \times log(|D|)$ with $|D|$ tuples. The proof is left as an exercise for the reader.

Incremental versions of decision tree induction have also been proposed. When given new training data, these restructure the decision tree acquired from learning on previous training data, rather than relearning a new tree from scratch.

Differences in decision tree algorithms include how the attributes are selected in creating the tree (Section 8.2.2) and the mechanisms used for pruning (Section 8.2.3). The basic algorithm described earlier requires one pass over the training tuples in D for each level of the tree. This can lead to long training times and lack of available memory when dealing with large databases. Improvements regarding the scalability of decision tree induction are discussed in Section 8.2.4. Section 8.2.5 presents a visual interactive approach to decision tree construction. A discussion of strategies for extracting rules from decision trees is given in Section 8.4.2 regarding rule-based classification.

8.2.2 Attribute Selection Measures

An **attribute selection measure** is a heuristic for selecting the splitting criterion that "best" separates a given data partition, D, of class-labeled training tuples into individual classes. If we were to split D into smaller partitions according to the outcomes of the splitting criterion, ideally each partition would be pure (i.e., all the tuples that fall into a given partition would belong to the same class). Conceptually, the "best" splitting criterion is the one that most closely results in such a scenario. Attribute selection measures are also known as **splitting rules** because they determine how the tuples at a given node are to be split.

The attribute selection measure provides a ranking for each attribute describing the given training tuples. The attribute having the best score for the measure[4] is chosen as the *splitting attribute* for the given tuples. If the splitting attribute is continuous-valued or if we are restricted to binary trees, then, respectively, either a *split point* or a *splitting subset* must also be determined as part of the splitting criterion. The tree node created for partition D is labeled with the splitting criterion, branches are grown for each outcome of the criterion, and the tuples are partitioned accordingly. This section describes three popular attribute selection measures—*information gain, gain ratio*, and *Gini index*.

The notation used herein is as follows. Let D, the data partition, be a training set of class-labeled tuples. Suppose the class label attribute has m distinct values defining m distinct classes, C_i (for $i = 1, \ldots, m$). Let $C_{i,D}$ be the set of tuples of class C_i in D. Let $|D|$ and $|C_{i,D}|$ denote the number of tuples in D and $C_{i,D}$, respectively.

Information Gain

ID3 uses **information gain** as its attribute selection measure. This measure is based on pioneering work by Claude Shannon on information theory, which studied the value or "information content" of messages. Let node N represent or hold the tuples of partition D. The attribute with the highest information gain is chosen as the splitting attribute for node N. This attribute minimizes the information needed to classify the tuples in the

[4]Depending on the measure, either the highest or lowest score is chosen as the best (i.e., some measures strive to maximize while others strive to minimize).

resulting partitions and reflects the least randomness or "impurity" in these partitions. Such an approach minimizes the expected number of tests needed to classify a given tuple and guarantees that a simple (but not necessarily the simplest) tree is found.

The expected information needed to classify a tuple in D is given by

$$Info(D) = -\sum_{i=1}^{m} p_i \log_2(p_i), \tag{8.1}$$

where p_i is the nonzero probability that an arbitrary tuple in D belongs to class C_i and is estimated by $|C_{i,D}|/|D|$. A log function to the base 2 is used, because the information is encoded in bits. $Info(D)$ is just the average amount of information needed to identify the class label of a tuple in D. Note that, at this point, the information we have is based solely on the proportions of tuples of each class. $Info(D)$ is also known as the **entropy** of D.

Now, suppose we were to partition the tuples in D on some attribute A having v distinct values, $\{a_1, a_2, \ldots, a_v\}$, as observed from the training data. If A is discrete-valued, these values correspond directly to the v outcomes of a test on A. Attribute A can be used to split D into v partitions or subsets, $\{D_1, D_2, \ldots, D_v\}$, where D_j contains those tuples in D that have outcome a_j of A. These partitions would correspond to the branches grown from node N. Ideally, we would like this partitioning to produce an exact classification of the tuples. That is, we would like for each partition to be pure. However, it is quite likely that the partitions will be impure (e.g., where a partition may contain a collection of tuples from different classes rather than from a single class).

How much more information would we still need (after the partitioning) to arrive at an exact classification? This amount is measured by

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times Info(D_j). \tag{8.2}$$

The term $\frac{|D_j|}{|D|}$ acts as the weight of the jth partition. $Info_A(D)$ is the expected information required to classify a tuple from D based on the partitioning by A. The smaller the expected information (still) required, the greater the purity of the partitions.

Information gain is defined as the difference between the original information requirement (i.e., based on just the proportion of classes) and the new requirement (i.e., obtained after partitioning on A). That is,

$$Gain(A) = Info(D) - Info_A(D). \tag{8.3}$$

In other words, $Gain(A)$ tells us how much would be gained by branching on A. It is the expected reduction in the information requirement caused by knowing the value of A. The attribute A with the highest information gain, $Gain(A)$, is chosen as the splitting attribute at node N. This is equivalent to saying that we want to partition on the attribute A that would do the "best classification," so that the amount of information still required to finish classifying the tuples is minimal (i.e., minimum $Info_A(D)$).

Table 8.1 Class-Labeled Training Tuples from the *AllElectronics* Customer Database

RID	*age*	*income*	*student*	*credit_rating*	*Class: buys_computer*
1	youth	high	no	fair	no
2	youth	high	no	excellent	no
3	middle_aged	high	no	fair	yes
4	senior	medium	no	fair	yes
5	senior	low	yes	fair	yes
6	senior	low	yes	excellent	no
7	middle_aged	low	yes	excellent	yes
8	youth	medium	no	fair	no
9	youth	low	yes	fair	yes
10	senior	medium	yes	fair	yes
11	youth	medium	yes	excellent	yes
12	middle_aged	medium	no	excellent	yes
13	middle_aged	high	yes	fair	yes
14	senior	medium	no	excellent	no

Example 8.1 **Induction of a decision tree using information gain.** Table 8.1 presents a training set, D, of class-labeled tuples randomly selected from the *AllElectronics* customer database. (The data are adapted from Quinlan [Qui86]. In this example, each attribute is discrete-valued. Continuous-valued attributes have been generalized.) The class label attribute, *buys_computer*, has two distinct values (namely, {*yes*, *no*}); therefore, there are two distinct classes (i.e., $m = 2$). Let class C_1 correspond to *yes* and class C_2 correspond to *no*. There are nine tuples of class *yes* and five tuples of class *no*. A (root) node N is created for the tuples in D. To find the splitting criterion for these tuples, we must compute the information gain of each attribute. We first use Eq. (8.1) to compute the expected information needed to classify a tuple in D:

$$Info(D) = -\frac{9}{14}\log_2\left(\frac{9}{14}\right) - \frac{5}{14}\log_2\left(\frac{5}{14}\right) = 0.940 \text{ bits.}$$

Next, we need to compute the expected information requirement for each attribute. Let's start with the attribute *age*. We need to look at the distribution of *yes* and *no* tuples for each category of *age*. For the *age* category "youth," there are two *yes* tuples and three *no* tuples. For the category "middle_aged," there are four *yes* tuples and zero *no* tuples. For the category "senior," there are three *yes* tuples and two *no* tuples. Using Eq. (8.2), the expected information needed to classify a tuple in D if the tuples are partitioned according to *age* is

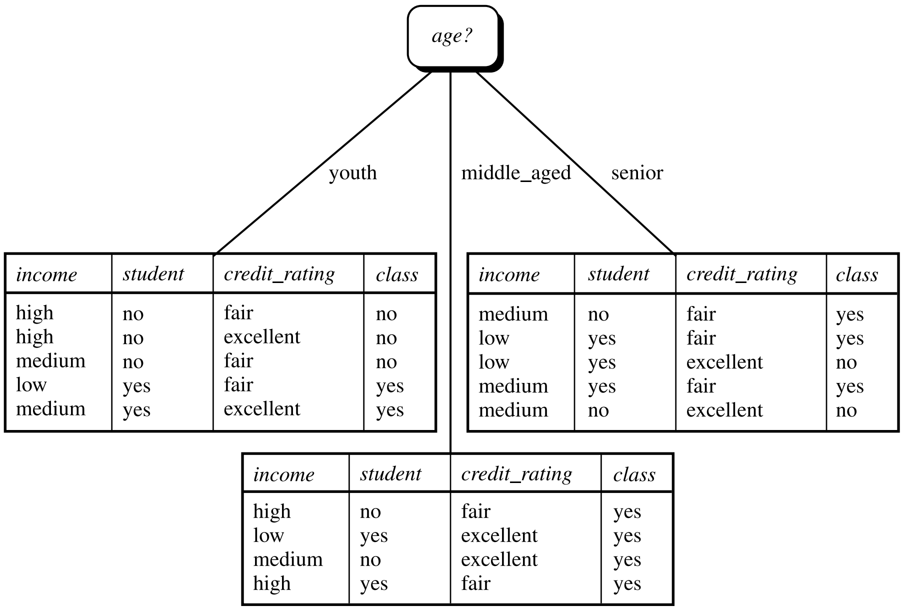
$$Info_{age}(D) = \frac{5}{14} \times \left(-\frac{2}{5}\log_2\frac{2}{5} - \frac{3}{5}\log_2\frac{3}{5}\right)$$

$$
\begin{aligned}
&+\frac{4}{14}\times\left(-\frac{4}{4}\log_2\frac{4}{4}\right)\\
&+\frac{5}{14}\times\left(-\frac{3}{5}\log_2\frac{3}{5}-\frac{2}{5}\log_2\frac{2}{5}\right)\\
&=0.694 \text{ bits.}
\end{aligned}
$$

Hence, the gain in information from such a partitioning would be

$$Gain(age) = Info(D) - Info_{age}(D) = 0.940 - 0.694 = 0.246 \text{ bits.}$$

Similarly, we can compute $Gain(income) = 0.029$ bits, $Gain(student) = 0.151$ bits, and $Gain(credit\_rating) = 0.048$ bits. Because *age* has the highest information gain among the attributes, it is selected as the splitting attribute. Node N is labeled with *age*, and branches are grown for each of the attribute's values. The tuples are then partitioned accordingly, as shown in Figure 8.5. Notice that the tuples falling into the partition for $age = middle\_aged$ all belong to the same class. Because they all belong to class *"yes,"* a leaf should therefore be created at the end of this branch and labeled *"yes."* The final decision tree returned by the algorithm was shown earlier in Figure 8.2. ■



income	*student*	*credit_rating*	*class*
high	no	fair	no
high	no	excellent	no
medium	no	fair	no
low	yes	fair	yes
medium	yes	excellent	yes

income	*student*	*credit_rating*	*class*
high	no	fair	yes
low	yes	excellent	yes
medium	no	excellent	yes
high	yes	fair	yes

income	*student*	*credit_rating*	*class*
medium	no	fair	yes
low	yes	fair	yes
low	yes	excellent	no
medium	yes	fair	yes
medium	no	excellent	no

Figure 8.5 The attribute *age* has the highest information gain and therefore becomes the splitting attribute at the root node of the decision tree. Branches are grown for each outcome of *age*. The tuples are shown partitioned accordingly.

"But how can we compute the information gain of an attribute that is continuous-valued, unlike in the example?" Suppose, instead, that we have an attribute A that is continuous-valued, rather than discrete-valued. (For example, suppose that instead of the discretized version of *age* from the example, we have the raw values for this attribute.) For such a scenario, we must determine the "best" **split-point** for A, where the split-point is a threshold on A.

We first sort the values of A in increasing order. Typically, the midpoint between each pair of adjacent values is considered as a possible split-point. Therefore, given v values of A, then $v-1$ possible splits are evaluated. For example, the midpoint between the values a_i and a_{i+1} of A is

$$\frac{a_i + a_{i+1}}{2}. \tag{8.4}$$

If the values of A are sorted in advance, then determining the best split for A requires only one pass through the values. For each possible split-point for A, we evaluate $Info_A(D)$, where the number of partitions is two, that is, $v = 2$ (or $j = 1, 2$) in Eq. (8.2). The point with the minimum expected information requirement for A is selected as the *split_point* for A. D_1 is the set of tuples in D satisfying $A \leq split\_point$, and D_2 is the set of tuples in D satisfying $A > split\_point$.

Gain Ratio

The information gain measure is biased toward tests with many outcomes. That is, it prefers to select attributes having a large number of values. For example, consider an attribute that acts as a unique identifier such as *product_ID*. A split on *product_ID* would result in a large number of partitions (as many as there are values), each one containing just one tuple. Because each partition is pure, the information required to classify data set D based on this partitioning would be $Info_{product\_ID}(D) = 0$. Therefore, the information gained by partitioning on this attribute is maximal. Clearly, such a partitioning is useless for classification.

C4.5, a successor of ID3, uses an extension to information gain known as *gain ratio*, which attempts to overcome this bias. It applies a kind of normalization to information gain using a "split information" value defined analogously with $Info(D)$ as

$$SplitInfo_A(D) = -\sum_{j=1}^{v} \frac{|D_j|}{|D|} \times \log_2\left(\frac{|D_j|}{|D|}\right). \tag{8.5}$$

This value represents the potential information generated by splitting the training data set, D, into v partitions, corresponding to the v outcomes of a test on attribute A. Note that, for each outcome, it considers the number of tuples having that outcome with respect to the total number of tuples in D. It differs from information gain, which measures the information with respect to classification that is acquired based on the same partitioning. The gain ratio is defined as

$$GainRatio(A) = \frac{Gain(A)}{SplitInfo_A(D)}. \tag{8.6}$$

The attribute with the maximum gain ratio is selected as the splitting attribute. Note, however, that as the split information approaches 0, the ratio becomes unstable. A constraint is added to avoid this, whereby the information gain of the test selected must be large—at least as great as the average gain over all tests examined.

Example 8.2 **Computation of gain ratio for the attribute *income*.** A test on *income* splits the data of Table 8.1 into three partitions, namely *low*, *medium*, and *high*, containing four, six, and four tuples, respectively. To compute the gain ratio of *income*, we first use Eq. (8.5) to obtain

$$\begin{aligned} SplitInfo_{income}(D) &= -\frac{4}{14} \times \log_2\left(\frac{4}{14}\right) - \frac{6}{14} \times \log_2\left(\frac{6}{14}\right) - \frac{4}{14} \times \log_2\left(\frac{4}{14}\right) \\ &= 1.557. \end{aligned}$$

From Example 8.1, we have $Gain(income) = 0.029$. Therefore, $GainRatio(income) = 0.029/1.557 = 0.019$. ■

Gini Index

The Gini index is used in CART. Using the notation previously described, the Gini index measures the impurity of D, a data partition or set of training tuples, as

$$Gini(D) = 1 - \sum_{i=1}^{m} p_i^2, \tag{8.7}$$

where p_i is the probability that a tuple in D belongs to class C_i and is estimated by $|C_{i,D}|/|D|$. The sum is computed over m classes.

The Gini index considers a binary split for each attribute. Let's first consider the case where A is a discrete-valued attribute having v distinct values, $\{a_1, a_2, \ldots, a_v\}$, occurring in D. To determine the best binary split on A, we examine all the possible subsets that can be formed using known values of A. Each subset, S_A, can be considered as a binary test for attribute A of the form "$A \in S_A$?" Given a tuple, this test is satisfied if the value of A for the tuple is among the values listed in S_A. If A has v possible values, then there are 2^v possible subsets. For example, if *income* has three possible values, namely {*low, medium, high*}, then the possible subsets are {*low, medium, high*}, {*low, medium*}, {*low, high*}, {*medium, high*}, {*low*}, {*medium*}, {*high*}, and {}. We exclude the power set, {*low, medium, high*}, and the empty set from consideration since, conceptually, they do not represent a split. Therefore, there are $2^v - 2$ possible ways to form two partitions of the data, D, based on a binary split on A.

When considering a binary split, we compute a weighted sum of the impurity of each resulting partition. For example, if a binary split on A partitions D into D_1 and D_2, the Gini index of D given that partitioning is

$$Gini_A(D) = \frac{|D_1|}{|D|} Gini(D_1) + \frac{|D_2|}{|D|} Gini(D_2). \tag{8.8}$$

For each attribute, each of the possible binary splits is considered. For a discrete-valued attribute, the subset that gives the minimum Gini index for that attribute is selected as its splitting subset.

For continuous-valued attributes, each possible split-point must be considered. The strategy is similar to that described earlier for information gain, where the midpoint between each pair of (sorted) adjacent values is taken as a possible split-point. The point giving the minimum Gini index for a given (continuous-valued) attribute is taken as the split-point of that attribute. Recall that for a possible split-point of A, D_1 is the set of tuples in D satisfying $A \leq split\_point$, and D_2 is the set of tuples in D satisfying $A > split\_point$.

The reduction in impurity that would be incurred by a binary split on a discrete- or continuous-valued attribute A is

$$\Delta Gini(A) = Gini(D) - Gini_A(D). \tag{8.9}$$

The attribute that maximizes the reduction in impurity (or, equivalently, has the minimum Gini index) is selected as the splitting attribute. This attribute and either its splitting subset (for a discrete-valued splitting attribute) or split-point (for a continuous-valued splitting attribute) together form the splitting criterion.

Example 8.3 **Induction of a decision tree using the Gini index.** Let D be the training data shown earlier in Table 8.1, where there are nine tuples belonging to the class $buys\_computer = yes$ and the remaining five tuples belong to the class $buys\_computer = no$. A (root) node N is created for the tuples in D. We first use Eq. (8.7) for the Gini index to compute the impurity of D:

$$Gini(D) = 1 - \left(\frac{9}{14}\right)^2 - \left(\frac{5}{14}\right)^2 = 0.459.$$

To find the splitting criterion for the tuples in D, we need to compute the Gini index for each attribute. Let's start with the attribute *income* and consider each of the possible splitting subsets. Consider the subset {*low, medium*}. This would result in 10 tuples in partition D_1 satisfying the condition "*income* ∈ {*low, medium*}." The remaining four tuples of D would be assigned to partition D_2. The Gini index value computed based on this partitioning is

$$
\begin{aligned}
&Gini_{income \in \{low, medium\}}(D) \\
&\quad = \frac{10}{14} Gini(D_1) + \frac{4}{14} Gini(D_2) \\
&\quad = \frac{10}{14}\left(1 - \left(\frac{7}{10}\right)^2 - \left(\frac{3}{10}\right)^2\right) + \frac{4}{14}\left(1 - \left(\frac{2}{4}\right)^2 - \left(\frac{2}{4}\right)^2\right) \\
&\quad = 0.443 \\
&\quad = Gini_{income \in \{high\}}(D).
\end{aligned}
$$

Similarly, the Gini index values for splits on the remaining subsets are 0.458 (for the subsets {*low, high*} and {*medium*}) and 0.450 (for the subsets {*medium, high*} and {*low*}). Therefore, the best binary split for attribute *income* is on {*low, medium*} (or {*high*}) because it minimizes the Gini index. Evaluating *age*, we obtain {*youth, senior*} (or {*middle_aged*}) as the best split for *age* with a Gini index of 0.375; the attributes *student* and *credit_rating* are both binary, with Gini index values of 0.367 and 0.429, respectively.

The attribute *age* and splitting subset {*youth, senior*} therefore give the minimum Gini index overall, with a reduction in impurity of $0.459 - 0.357 = 0.102$. The binary split "*age* ∈ {*youth, senior*?}" results in the maximum reduction in impurity of the tuples in D and is returned as the splitting criterion. Node N is labeled with the criterion, two branches are grown from it, and the tuples are partitioned accordingly. ■

Other Attribute Selection Measures

This section on attribute selection measures was not intended to be exhaustive. We have shown three measures that are commonly used for building decision trees. These measures are not without their biases. Information gain, as we saw, is biased toward multivalued attributes. Although the gain ratio adjusts for this bias, it tends to prefer unbalanced splits in which one partition is much smaller than the others. The Gini index is biased toward multivalued attributes and has difficulty when the number of classes is large. It also tends to favor tests that result in equal-size partitions and purity in both partitions. Although biased, these measures give reasonably good results in practice.

Many other attribute selection measures have been proposed. CHAID, a decision tree algorithm that is popular in marketing, uses an attribute selection measure that is based on the statistical χ^2 test for independence. Other measures include C-SEP (which performs better than information gain and the Gini index in certain cases) and G-statistic (an information theoretic measure that is a close approximation to χ^2 distribution).

Attribute selection measures based on the **Minimum Description Length (MDL)** principle have the least bias toward multivalued attributes. MDL-based measures use encoding techniques to define the "best" decision tree as the one that requires the fewest number of bits to both (1) encode the tree and (2) encode the exceptions to the tree (i.e., cases that are not correctly classified by the tree). Its main idea is that the simplest of solutions is preferred.

Other attribute selection measures consider **multivariate splits** (i.e., where the partitioning of tuples is based on a *combination* of attributes, rather than on a single attribute). The CART system, for example, can find multivariate splits based on a linear combination of attributes. Multivariate splits are a form of **attribute** (or feature) **construction**, where new attributes are created based on the existing ones. (Attribute construction was also discussed in Chapter 3, as a form of data transformation.) These other measures mentioned here are beyond the scope of this book. Additional references are given in the bibliographic notes at the end of this chapter (Section 8.9).

"Which attribute selection measure is the best?" All measures have some bias. It has been shown that the time complexity of decision tree induction generally increases exponentially with tree height. Hence, measures that tend to produce shallower trees (e.g., with multiway rather than binary splits, and that favor more balanced splits) may be preferred. However, some studies have found that shallow trees tend to have a large number of leaves and higher error rates. Despite several comparative studies, no one attribute selection measure has been found to be significantly superior to others. Most measures give quite good results.

8.2.3 Tree Pruning

When a decision tree is built, many of the branches will reflect anomalies in the training data due to noise or outliers. Tree pruning methods address this problem of *overfitting* the data. Such methods typically use statistical measures to remove the least-reliable branches. An unpruned tree and a pruned version of it are shown in Figure 8.6. Pruned trees tend to be smaller and less complex and, thus, easier to comprehend. They are usually faster and better at correctly classifying independent test data (i.e., of previously unseen tuples) than unpruned trees.

"How does tree pruning work?" There are two common approaches to tree pruning: *prepruning* and *postpruning*.

In the **prepruning** approach, a tree is "pruned" by halting its construction early (e.g., by deciding not to further split or partition the subset of training tuples at a given node). Upon halting, the node becomes a leaf. The leaf may hold the most frequent class among the subset tuples or the probability distribution of those tuples.

When constructing a tree, measures such as statistical significance, information gain, Gini index, and so on, can be used to assess the goodness of a split. If partitioning the tuples at a node would result in a split that falls below a prespecified threshold, then further partitioning of the given subset is halted. There are difficulties, however, in choosing an appropriate threshold. High thresholds could result in oversimplified trees, whereas low thresholds could result in very little simplification.

The second and more common approach is **postpruning**, which removes subtrees from a "fully grown" tree. A subtree at a given node is pruned by removing its branches and replacing it with a leaf. The leaf is labeled with the most frequent class among the subtree being replaced. For example, notice the subtree at node "A_3?" in the unpruned

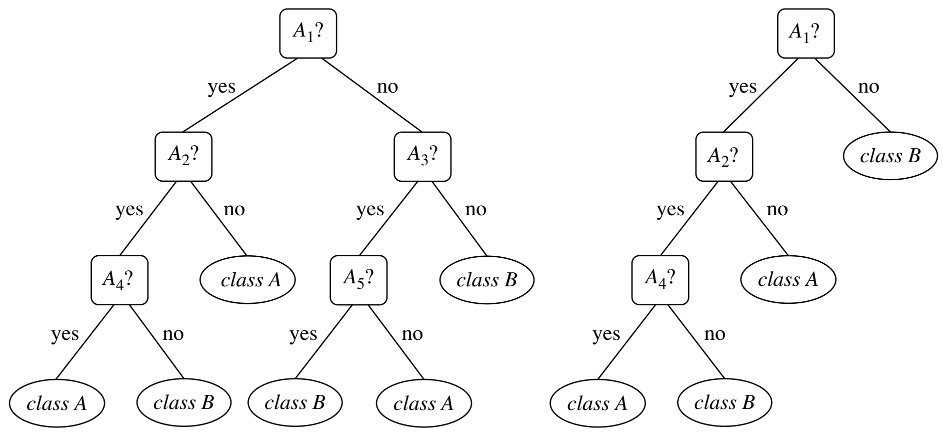


Figure 8.6 An unpruned decision tree and a pruned version of it.

tree of Figure 8.6. Suppose that the most common class within this subtree is "*class B*." In the pruned version of the tree, the subtree in question is pruned by replacing it with the leaf "*class B*."

The **cost complexity** pruning algorithm used in CART is an example of the postpruning approach. This approach considers the cost complexity of a tree to be a function of the number of leaves in the tree and the error rate of the tree (where the **error rate** is the percentage of tuples misclassified by the tree). It starts from the bottom of the tree. For each internal node, N, it computes the cost complexity of the subtree at N, and the cost complexity of the subtree at N if it were to be pruned (i.e., replaced by a leaf node). The two values are compared. If pruning the subtree at node N would result in a smaller cost complexity, then the subtree is pruned. Otherwise, it is kept.

A **pruning set** of class-labeled tuples is used to estimate cost complexity. This set is independent of the training set used to build the unpruned tree and of any test set used for accuracy estimation. The algorithm generates a set of progressively pruned trees. In general, the smallest decision tree that minimizes the cost complexity is preferred.

C4.5 uses a method called **pessimistic pruning**, which is similar to the cost complexity method in that it also uses error rate estimates to make decisions regarding subtree pruning. Pessimistic pruning, however, does not require the use of a prune set. Instead, it uses the training set to estimate error rates. Recall that an estimate of accuracy or error based on the training set is overly optimistic and, therefore, strongly biased. The pessimistic pruning method therefore adjusts the error rates obtained from the training set by adding a penalty, so as to counter the bias incurred.

Rather than pruning trees based on estimated error rates, we can prune trees based on the number of bits required to encode them. The "best" pruned tree is the one that minimizes the number of encoding bits. This method adopts the MDL principle, which was briefly introduced in Section 8.2.2. The basic idea is that the simplest solution is preferred. Unlike cost complexity pruning, it does not require an independent set of tuples.

Alternatively, prepruning and postpruning may be interleaved for a combined approach. Postpruning requires more computation than prepruning, yet generally leads to a more reliable tree. No single pruning method has been found to be superior over all others. Although some pruning methods do depend on the availability of additional data for pruning, this is usually not a concern when dealing with large databases.

Although pruned trees tend to be more compact than their unpruned counterparts, they may still be rather large and complex. Decision trees can suffer from *repetition* and *replication* (Figure 8.7), making them overwhelming to interpret. **Repetition** occurs when an attribute is repeatedly tested along a given branch of the tree (e.g., "*age* < *60?*,"

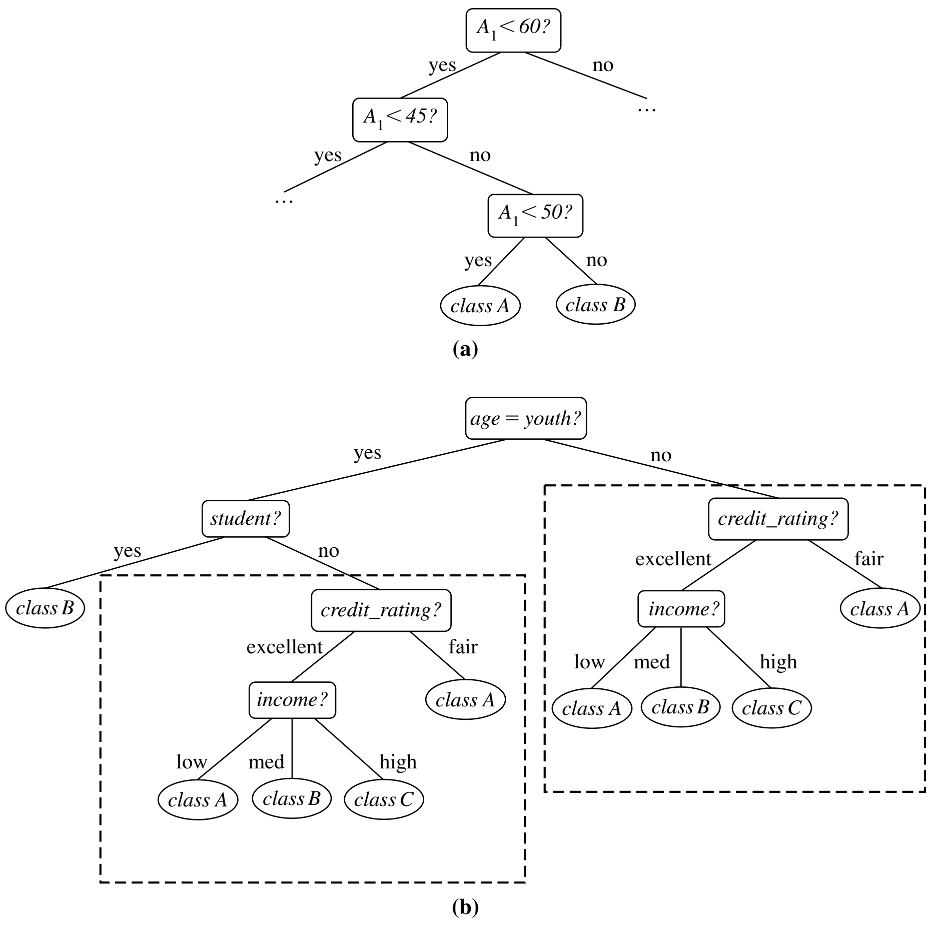


Figure 8.7 An example of: (a) subtree **repetition**, where an attribute is repeatedly tested along a given branch of the tree (e.g., *age*) and (b) subtree **replication**, where duplicate subtrees exist within a tree (e.g., the subtree headed by the node "*credit_rating?*").

followed by *"age < 45?,"* and so on). In **replication**, duplicate subtrees exist within the tree. These situations can impede the accuracy and comprehensibility of a decision tree. The use of multivariate splits (splits based on a combination of attributes) can prevent these problems. Another approach is to use a different form of knowledge representation, such as rules, instead of decision trees. This is described in Section 8.4.2, which shows how a *rule-based classifier* can be constructed by extracting IF-THEN rules from a decision tree.

8.2.4 Scalability and Decision Tree Induction

"What if D, the disk-resident training set of class-labeled tuples, does not fit in memory? In other words, how scalable is decision tree induction?" The efficiency of existing decision tree algorithms, such as ID3, C4.5, and CART, has been well established for relatively small data sets. Efficiency becomes an issue of concern when these algorithms are applied to the mining of very large real-world databases. The pioneering decision tree algorithms that we have discussed so far have the restriction that the training tuples should reside *in memory*.

In data mining applications, very large training sets of millions of tuples are common. Most often, the training data will not fit in memory! Therefore, decision tree construction becomes inefficient due to swapping of the training tuples in and out of main and cache memories. More scalable approaches, capable of handling training data that are too large to fit in memory, are required. Earlier strategies to "save space" included discretizing continuous-valued attributes and sampling data at each node. These techniques, however, still assume that the training set can fit in memory.

Several scalable decision tree induction methods have been introduced in recent studies. RainForest, for example, adapts to the amount of main memory available and applies to any decision tree induction algorithm. The method maintains an **AVC-set** (where "AVC" stands for "*Attribute-Value*, *Classlabel*") for each attribute, at each tree node, describing the training tuples at the node. The AVC-set of an attribute A at node N gives the class label counts for each value of A for the tuples at N. Figure 8.8 shows AVC-sets for the tuple data of Table 8.1. The set of all AVC-sets at a node N is the **AVC-group** of N. The size of an AVC-set for attribute A at node N depends only on the number of distinct values of A and the number of classes in the set of tuples at N. Typically, this size should fit in memory, even for real-world data. RainForest also has techniques, however, for handling the case where the AVC-group does not fit in memory. Therefore, the method has high scalability for decision tree induction in very large data sets.

BOAT (Bootstrapped Optimistic Algorithm for Tree construction) is a decision tree algorithm that takes a completely different approach to scalability—it is not based on the use of any special data structures. Instead, it uses a statistical technique known as "bootstrapping" (Section 8.5.4) to create several smaller samples (or subsets) of the given training data, each of which fits in memory. Each subset is used to construct a tree, resulting in several trees. The trees are examined and used to construct a new tree, T', that turns out to be "very close" to the tree that would have been generated if all the original training data had fit in memory.

	buys_computer	
age	yes	no
youth	2	3
middle_aged	4	0
senior	3	2

	buys_computer	
income	yes	no
low	3	1
medium	4	2
high	2	2

	buys_computer	
student	yes	no
yes	6	1
no	3	4

	buys_computer	
credit_ratting	yes	no
fair	6	2
excellent	3	3

Figure 8.8 The use of data structures to hold aggregate information regarding the training data (e.g., these AVC-sets describing Table 8.1's data) are one approach to improving the scalability of decision tree induction.

BOAT can use any attribute selection measure that selects binary splits and that is based on the notion of purity of partitions such as the Gini index. BOAT uses a lower bound on the attribute selection measure to detect if this "very good" tree, T', is different from the "real" tree, T, that would have been generated using all of the data. It refines T' to arrive at T.

BOAT usually requires only two scans of D. This is quite an improvement, even in comparison to traditional decision tree algorithms (e.g., the basic algorithm in Figure 8.3), which require one scan per tree level! BOAT was found to be two to three times faster than RainForest, while constructing exactly the same tree. An additional advantage of BOAT is that it can be used for incremental updates. That is, BOAT can take new insertions and deletions for the training data and update the decision tree to reflect these changes, without having to reconstruct the tree from scratch.

8.2.5 Visual Mining for Decision Tree Induction

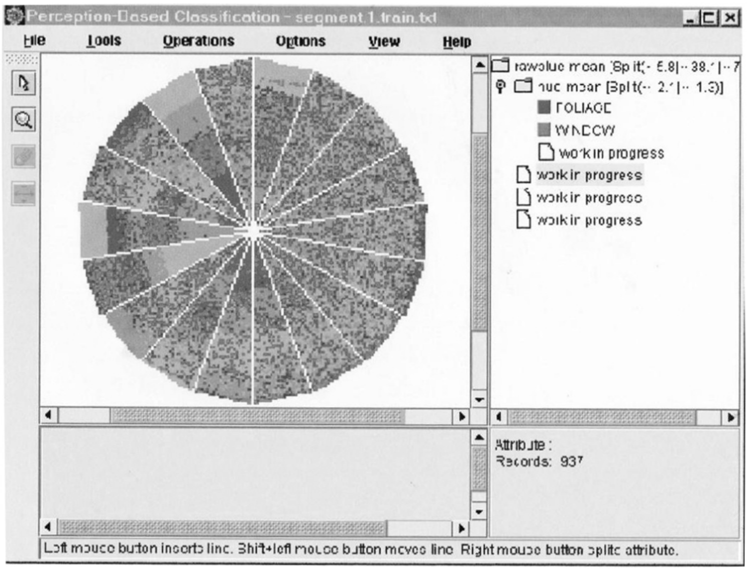
"Are there any interactive approaches to decision tree induction that allow us to visualize the data and the tree as it is being constructed? Can we use any knowledge of our data to help in building the tree?" In this section, you will learn about an approach to decision tree induction that supports these options. **Perception-based classification (PBC)** is an interactive approach based on multidimensional visualization techniques and allows the user to incorporate background knowledge about the data when building a decision tree. By visually interacting with the data, the user is also likely to develop a deeper understanding of the data. The resulting trees tend to be smaller than those built using traditional decision tree induction methods and so are easier to interpret, while achieving about the same accuracy.

"How can the data be visualized to support interactive decision tree construction?" PBC uses a pixel-oriented approach to view multidimensional data with its class label

information. The circle segments approach is adapted, which maps d-dimensional data objects to a circle that is partitioned into d segments, each representing one attribute (Section 2.3.1). Here, an attribute value of a data object is mapped to one colored pixel, reflecting the object's class label. This mapping is done for each attribute–value pair of each data object. Sorting is done for each attribute to determine the arrangement order within a segment. For example, attribute values within a given segment may be organized so as to display homogeneous (with respect to class label) regions within the same attribute value. The amount of training data that can be visualized at one time is approximately determined by the product of the number of attributes and the number of data objects.

The PBC system displays a split screen, consisting of a Data Interaction window and a Knowledge Interaction window (Figure 8.9). The Data Interaction window displays the circle segments of the data under examination, while the Knowledge Interaction window displays the decision tree constructed so far. Initially, the complete training set is visualized in the Data Interaction window, while the Knowledge Interaction window displays an empty decision tree.

Traditional decision tree algorithms allow only binary splits for numeric attributes. PBC, however, allows the user to specify multiple split-points, resulting in multiple branches to be grown from a single tree node.



rawvalue mean [Split(-- 6.8|-- 38.1|-- 7
hue mean [Split(-- 2.1|-- 1.3)]
FOLIAGE
WINDOW
work in progress
work in progress
work in progress
work in progress

Attribute :
Records: 937

Left mouse button inserts line. Shift+left mouse button moves line. Right mouse button splits attribute.

Figure 8.9 A screenshot of PBC, a system for interactive decision tree construction. Multidimensional training data are viewed as circle segments in the Data Interaction window (*left*). The Knowledge Interaction window (*right*) displays the current decision tree. *Source:* From Ankerst, Elsen, Ester, and Kriegel [AEEK99].

A tree is interactively constructed as follows. The user visualizes the multidimensional data in the Data Interaction window and selects a splitting attribute and one or more split-points. The current decision tree in the Knowledge Interaction window is expanded. The user selects a node of the decision tree. The user may either assign a class label to the node (which makes the node a leaf) or request the visualization of the training data corresponding to the node. This leads to a new visualization of every attribute except the ones used for splitting criteria on the same path from the root. The interactive process continues until a class has been assigned to each leaf of the decision tree.

The trees constructed with PBC were compared with trees generated by the CART, C4.5, and SPRINT algorithms from various data sets. The trees created with PBC were of comparable accuracy with the tree from the algorithmic approaches, yet were significantly smaller and, thus, easier to understand. Users can use their domain knowledge in building a decision tree, but also gain a deeper understanding of their data during the construction process.

8.3 Bayes Classification Methods

"What are Bayesian classifiers?" Bayesian classifiers are statistical classifiers. They can predict class membership probabilities such as the probability that a given tuple belongs to a particular class.

Bayesian classification is based on Bayes' theorem, described next. Studies comparing classification algorithms have found a simple Bayesian classifier known as the *naïve Bayesian classifier* to be comparable in performance with decision tree and selected neural network classifiers. Bayesian classifiers have also exhibited high accuracy and speed when applied to large databases.

Naïve Bayesian classifiers assume that the effect of an attribute value on a given class is independent of the values of the other attributes. This assumption is called *class-conditional independence*. It is made to simplify the computations involved and, in this sense, is considered "naïve."

Section 8.3.1 reviews basic probability notation and Bayes' theorem. In Section 8.3.2 you will learn how to do naïve Bayesian classification.

8.3.1 Bayes' Theorem

Bayes' theorem is named after Thomas Bayes, a nonconformist English clergyman who did early work in probability and decision theory during the 18th century. Let $\boldsymbol{X}$ be a data tuple. In Bayesian terms, $\boldsymbol{X}$ is considered "evidence." As usual, it is described by measurements made on a set of n attributes. Let H be some hypothesis such as that the data tuple $\boldsymbol{X}$ belongs to a specified class C. For classification problems, we want to determine $P(H|\boldsymbol{X})$, the probability that the hypothesis H holds given the "evidence" or observed data tuple $\boldsymbol{X}$. In other words, we are looking for the probability that tuple $\boldsymbol{X}$ belongs to class C, given that we know the attribute description of $\boldsymbol{X}$.

$P(H|\boldsymbol{X})$ is the **posterior probability**, or *a posteriori probability*, of H conditioned on $\boldsymbol{X}$. For example, suppose our world of data tuples is confined to customers described by the attributes *age* and *income*, respectively, and that $\boldsymbol{X}$ is a 35-year-old customer with an income of \$40,000. Suppose that H is the hypothesis that our customer will buy a computer. Then $P(H|\boldsymbol{X})$ reflects the probability that customer $\boldsymbol{X}$ will buy a computer given that we know the customer's age and income.

In contrast, $P(H)$ is the **prior probability**, or *a priori probability*, of H. For our example, this is the probability that any given customer will buy a computer, regardless of age, income, or any other information, for that matter. The posterior probability, $P(H|\boldsymbol{X})$, is based on more information (e.g., customer information) than the prior probability, $P(H)$, which is independent of $\boldsymbol{X}$.

Similarly, $P(\boldsymbol{X}|H)$ is the posterior probability of $\boldsymbol{X}$ conditioned on H. That is, it is the probability that a customer, $\boldsymbol{X}$, is 35 years old and earns \$40,000, given that we know the customer will buy a computer.

$P(\boldsymbol{X})$ is the prior probability of $\boldsymbol{X}$. Using our example, it is the probability that a person from our set of customers is 35 years old and earns \$40,000.

"How are these probabilities estimated?" $P(H)$, $P(\boldsymbol{X}|H)$, and $P(\boldsymbol{X})$ may be estimated from the given data, as we shall see next. **Bayes' theorem** is useful in that it provides a way of calculating the posterior probability, $P(H|\boldsymbol{X})$, from $P(H)$, $P(\boldsymbol{X}|H)$, and $P(\boldsymbol{X})$. Bayes' theorem is

$$P(H|\boldsymbol{X}) = \frac{P(\boldsymbol{X}|H)P(H)}{P(\boldsymbol{X})}. \tag{8.10}$$

Now that we have that out of the way, in the next section, we will look at how Bayes' theorem is used in the naïve Bayesian classifier.

8.3.2 Naïve Bayesian Classification

The **naïve Bayesian** classifier, or **simple Bayesian** classifier, works as follows:

1. Let D be a training set of tuples and their associated class labels. As usual, each tuple is represented by an n-dimensional attribute vector, $\boldsymbol{X} = (x_1, x_2, \ldots, x_n)$, depicting n measurements made on the tuple from n attributes, respectively, $A_1, A_2, \ldots, A_n$.

2. Suppose that there are m classes, $C_1, C_2, \ldots, C_m$. Given a tuple, $\boldsymbol{X}$, the classifier will predict that $\boldsymbol{X}$ belongs to the class having the highest posterior probability, conditioned on $\boldsymbol{X}$. That is, the naïve Bayesian classifier predicts that tuple $\boldsymbol{X}$ belongs to the class C_i if and only if

$$P(C_i|\boldsymbol{X}) > P(C_j|\boldsymbol{X}) \quad \text{for } 1 \le j \le m, j \ne i.$$

Thus, we maximize $P(C_i|\boldsymbol{X})$. The class C_i for which $P(C_i|\boldsymbol{X})$ is maximized is called the *maximum posteriori hypothesis*. By Bayes' theorem (Eq. 8.10),

$$P(C_i|\boldsymbol{X}) = \frac{P(\boldsymbol{X}|C_i)P(C_i)}{P(\boldsymbol{X})}. \tag{8.11}$$

3. As $P(\boldsymbol{X})$ is constant for all classes, only $P(\boldsymbol{X}|C_i)P(C_i)$ needs to be maximized. If the class prior probabilities are not known, then it is commonly assumed that the classes are equally likely, that is, $P(C_1) = P(C_2) = \cdots = P(C_m)$, and we would therefore maximize $P(\boldsymbol{X}|C_i)$. Otherwise, we maximize $P(\boldsymbol{X}|C_i)P(C_i)$. Note that the class prior probabilities may be estimated by $P(C_i) = |C_{i,D}|/|D|$, where $|C_{i,D}|$ is the number of training tuples of class C_i in D.

4. Given data sets with many attributes, it would be extremely computationally expensive to compute $P(\boldsymbol{X}|C_i)$. To reduce computation in evaluating $P(\boldsymbol{X}|C_i)$, the naïve assumption of **class-conditional independence** is made. This presumes that the attributes' values are conditionally independent of one another, given the class label of the tuple (i.e., that there are no dependence relationships among the attributes). Thus,

$$P(\boldsymbol{X}|C_i) = \prod_{k=1}^{n} P(x_k|C_i) \tag{8.12}$$
$$= P(x_1|C_i) \times P(x_2|C_i) \times \cdots \times P(x_n|C_i).$$

We can easily estimate the probabilities $P(x_1|C_i), P(x_2|C_i), \ldots, P(x_n|C_i)$ from the training tuples. Recall that here x_k refers to the value of attribute A_k for tuple $\boldsymbol{X}$. For each attribute, we look at whether the attribute is categorical or continuous-valued. For instance, to compute $P(\boldsymbol{X}|C_i)$, we consider the following:

(a) If A_k is categorical, then $P(x_k|C_i)$ is the number of tuples of class C_i in D having the value x_k for A_k, divided by $|C_{i,D}|$, the number of tuples of class C_i in D.

(b) If A_k is continuous-valued, then we need to do a bit more work, but the calculation is pretty straightforward. A continuous-valued attribute is typically assumed to have a Gaussian distribution with a mean μ and standard deviation σ, defined by

$$g(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \tag{8.13}$$

so that

$$P(x_k|C_i) = g(x_k, \mu_{C_i}, \sigma_{C_i}). \tag{8.14}$$

These equations may appear daunting, but hold on! We need to compute μ_{C_i} and σ_{C_i}, which are the mean (i.e., average) and standard deviation, respectively, of the values of attribute A_k for training tuples of class C_i. We then plug these two quantities into Eq. (8.13), together with x_k, to estimate $P(x_k|C_i)$.

For example, let $\boldsymbol{X} = (35, \$40{,}000)$, where A_1 and A_2 are the attributes *age* and *income*, respectively. Let the class label attribute be *buys_computer*. The associated class label for $\boldsymbol{X}$ is *yes* (i.e., *buys_computer* = *yes*). Let's suppose that *age* has not been discretized and therefore exists as a continuous-valued attribute. Suppose that from the training set, we find that customers in D who buy a computer are

38 ± 12 years of age. In other words, for attribute *age* and this class, we have $\mu = 38$ years and $\sigma = 12$. We can plug these quantities, along with $x_1 = 35$ for our tuple $\boldsymbol{X}$, into Eq. (8.13) to estimate $P(age = 35 | buys\_computer = yes)$. For a quick review of mean and standard deviation calculations, please see Section 2.2.

5. To predict the class label of $\boldsymbol{X}$, $P(\boldsymbol{X}|C_i)P(C_i)$ is evaluated for each class C_i. The classifier predicts that the class label of tuple $\boldsymbol{X}$ is the class C_i if and only if

$$P(\boldsymbol{X}|C_i)P(C_i) > P(\boldsymbol{X}|C_j)P(C_j) \quad \text{for } 1 \leq j \leq m, j \neq i. \tag{8.15}$$

In other words, the predicted class label is the class C_i for which $P(\boldsymbol{X}|C_i)P(C_i)$ is the maximum.

"*How effective are Bayesian classifiers?*" Various empirical studies of this classifier in comparison to decision tree and neural network classifiers have found it to be comparable in some domains. In theory, Bayesian classifiers have the minimum error rate in comparison to all other classifiers. However, in practice this is not always the case, owing to inaccuracies in the assumptions made for its use, such as class-conditional independence, and the lack of available probability data.

Bayesian classifiers are also useful in that they provide a theoretical justification for other classifiers that do not explicitly use Bayes' theorem. For example, under certain assumptions, it can be shown that many neural network and curve-fitting algorithms output the *maximum posteriori* hypothesis, as does the naïve Bayesian classifier.

Example 8.4 **Predicting a class label using naïve Bayesian classification.** We wish to predict the class label of a tuple using naïve Bayesian classification, given the same training data as in Example 8.3 for decision tree induction. The training data were shown earlier in Table 8.1. The data tuples are described by the attributes *age*, *income*, *student*, and *credit_rating*. The class label attribute, *buys_computer*, has two distinct values (namely, {*yes*, *no*}). Let C_1 correspond to the class *buys_computer* = *yes* and C_2 correspond to *buys_computer* = *no*. The tuple we wish to classify is

$$\boldsymbol{X} = (age = youth,\ income = medium,\ student = yes,\ credit\_rating = fair)$$

We need to maximize $P(\boldsymbol{X}|C_i)P(C_i)$, for $i = 1, 2$. $P(C_i)$, the prior probability of each class, can be computed based on the training tuples:

$$P(buys\_computer = yes) = 9/14 = 0.643$$
$$P(buys\_computer = no) = 5/14 = 0.357$$

To compute $P(\boldsymbol{X}|C_i)$, for $i = 1, 2$, we compute the following conditional probabilities:

$$\begin{aligned}
P(age = youth \mid buys\_computer = yes) &= 2/9 = 0.222\\
P(age = youth \mid buys\_computer = no) &= 3/5 = 0.600\\
P(income = medium \mid buys\_computer = yes) &= 4/9 = 0.444\\
P(income = medium \mid buys\_computer = no) &= 2/5 = 0.400\\
P(student = yes \mid buys\_computer = yes) &= 6/9 = 0.667
\end{aligned}$$

$$\begin{aligned}
&P(student = yes \mid buys\_computer = no) &&= 1/5 = 0.200\\
&P(credit\_rating = fair \mid buys\_computer = yes) &&= 6/9 = 0.667\\
&P(credit\_rating = fair \mid buys\_computer = no) &&= 2/5 = 0.400
\end{aligned}$$

Using these probabilities, we obtain

$$\begin{aligned}
P(\boldsymbol{X}|buys\_computer = yes) &= P(age = youth \mid buys\_computer = yes)\\
&\quad\times P(income = medium \mid buys\_computer = yes)\\
&\quad\times P(student = yes \mid buys\_computer = yes)\\
&\quad\times P(credit\_rating = fair \mid buys\_computer = yes)\\
&= 0.222 \times 0.444 \times 0.667 \times 0.667 = 0.044.
\end{aligned}$$

Similarly,

$$P(\boldsymbol{X}|buys\_computer = no) = 0.600 \times 0.400 \times 0.200 \times 0.400 = 0.019.$$

To find the class, C_i, that maximizes $P(\boldsymbol{X}|C_i)P(C_i)$, we compute

$$\begin{aligned}
P(\boldsymbol{X}|buys\_computer = yes)P(buys\_computer = yes) &= 0.044 \times 0.643 = 0.028\\
P(\boldsymbol{X}|buys\_computer = no)P(buys\_computer = no) &= 0.019 \times 0.357 = 0.007
\end{aligned}$$

Therefore, the naïve Bayesian classifier predicts *buys_computer* = *yes* for tuple $\boldsymbol{X}$. ■

"*What if I encounter probability values of zero?*" Recall that in Eq. (8.12), we estimate $P(\boldsymbol{X}|C_i)$ as the product of the probabilities $P(x_1|C_i), P(x_2|C_i), \ldots, P(x_n|C_i)$, based on the assumption of class-conditional independence. These probabilities can be estimated from the training tuples (step 4). We need to compute $P(\boldsymbol{X}|C_i)$ for *each* class ($i = 1, 2, \ldots, m$) to find the class C_i for which $P(\boldsymbol{X}|C_i)P(C_i)$ is the maximum (step 5). Let's consider this calculation. For each attribute–value pair (i.e., $A_k = x_k$, for $k = 1, 2, \ldots, n$) in tuple $\boldsymbol{X}$, we need to count the number of tuples having that attribute–value pair, per class (i.e., per C_i, for $i = 1, \ldots, m$). In Example 8.4, we have two classes ($m = 2$), namely *buys_computer* = *yes* and *buys_computer* = *no*. Therefore, for the attribute–value pair *student* = *yes* of $\boldsymbol{X}$, say, we need two counts—the number of customers who are students and for which *buys_computer* = *yes* (which contributes to $P(\boldsymbol{X}|buys\_computer = yes)$) and the number of customers who are students and for which *buys_computer* = *no* (which contributes to $P(\boldsymbol{X}|buys\_computer = no)$).

But what if, say, there are no training tuples representing students for the class *buys_computer* = *no*, resulting in $P(student = yes|buys\_computer = no) = 0$? In other words, what happens if we should end up with a probability value of zero for some $P(x_k|C_i)$? Plugging this zero value into Eq. (8.12) would return a zero probability for $P(\boldsymbol{X}|C_i)$, even though, without the zero probability, we may have ended up with a high probability, suggesting that $\boldsymbol{X}$ belonged to class C_i! A zero probability cancels the effects of all the other (posteriori) probabilities (on C_i) involved in the product.

There is a simple trick to avoid this problem. We can assume that our training database, D, is so large that adding one to each count that we need would only make a negligible difference in the estimated probability value, yet would conveniently avoid the case of probability values of zero. This technique for probability estimation is known as the **Laplacian correction** or **Laplace estimator**, named after Pierre Laplace, a French mathematician who lived from 1749 to 1827. If we have, say, q counts to which we each add one, then we must remember to add q to the corresponding denominator used in the probability calculation. We illustrate this technique in Example 8.5.

Example 8.5 **Using the Laplacian correction to avoid computing probability values of zero.** Suppose that for the class *buys_computer* = *yes* in some training database, D, containing 1000 tuples, we have 0 tuples with *income* = *low*, 990 tuples with *income* = *medium*, and 10 tuples with *income* = *high*. The probabilities of these events, without the Laplacian correction, are 0, 0.990 (from 990/1000), and 0.010 (from 10/1000), respectively. Using the Laplacian correction for the three quantities, we pretend that we have 1 more tuple for each income-value pair. In this way, we instead obtain the following probabilities (rounded up to three decimal places):

$$\frac{1}{1003} = 0.001, \frac{991}{1003} = 0.988, \text{ and } \frac{11}{1003} = 0.011,$$

respectively. The "corrected" probability estimates are close to their "uncorrected" counterparts, yet the zero probability value is avoided. ■

8.4 Rule-Based Classification

In this section, we look at rule-based classifiers, where the learned model is represented as a set of IF-THEN rules. We first examine how such rules are used for classification (Section 8.4.1). We then study ways in which they can be generated, either from a decision tree (Section 8.4.2) or directly from the training data using a *sequential covering algorithm* (Section 8.4.3).

8.4.1 Using IF-THEN Rules for Classification

Rules are a good way of representing information or bits of knowledge. A **rule-based classifier** uses a set of IF-THEN rules for classification. An **IF-THEN** rule is an expression of the form

IF *condition* THEN *conclusion*.

An example is rule $R1$,

$R1$: IF *age* = *youth* AND *student* = *yes* THEN *buys_computer* = *yes*.

The "IF" part (or left side) of a rule is known as the **rule antecedent** or **precondition**. The "THEN" part (or right side) is the **rule consequent**. In the rule antecedent, the condition consists of one or more *attribute tests* (e.g., *age* = *youth* and *student* = *yes*) that are logically ANDed. The rule's consequent contains a class prediction (in this case, we are predicting whether a customer will buy a computer). $R1$ can also be written as

$$R1\text{: } (age = youth) \wedge (student = yes) \Rightarrow (buys\_computer = yes).$$

If the condition (i.e., all the attribute tests) in a rule antecedent holds true for a given tuple, we say that the rule antecedent is **satisfied** (or simply, that the rule is satisfied) and that the rule **covers** the tuple.

A rule R can be assessed by its coverage and accuracy. Given a tuple, $\boldsymbol{X}$, from a class-labeled data set, D, let n_{covers} be the number of tuples covered by R; $n_{correct}$ be the number of tuples correctly classified by R; and $|D|$ be the number of tuples in D. We can define the **coverage** and **accuracy** of R as

$$coverage(R) = \frac{n_{covers}}{|D|} \tag{8.16}$$

$$accuracy(R) = \frac{n_{correct}}{n_{covers}}. \tag{8.17}$$

That is, a rule's coverage is the percentage of tuples that are covered by the rule (i.e., their attribute values hold true for the rule's antecedent). For a rule's accuracy, we look at the tuples that it covers and see what percentage of them the rule can correctly classify.

Example 8.6 **Rule accuracy and coverage.** Let's go back to our data in Table 8.1. These are class-labeled tuples from the *AllElectronics* customer database. Our task is to predict whether a customer will buy a computer. Consider rule $R1$, which covers 2 of the 14 tuples. It can correctly classify both tuples. Therefore, $coverage(R1) = 2/14 = 14.28\%$ and $accuracy(R1) = 2/2 = 100\%$. ■

Let's see how we can use rule-based classification to predict the class label of a given tuple, $\boldsymbol{X}$. If a rule is satisfied by $\boldsymbol{X}$, the rule is said to be **triggered**. For example, suppose we have

$$\boldsymbol{X} = (age = youth,\ income = medium,\ student = yes,\ credit\_rating = fair).$$

We would like to classify $\boldsymbol{X}$ according to *buys_computer*. $\boldsymbol{X}$ satisfies $R1$, which triggers the rule.

If $R1$ is the only rule satisfied, then the rule **fires** by returning the class prediction for $\boldsymbol{X}$. Note that triggering does not always mean firing because there may be more than one rule that is satisfied! If more than one rule is triggered, we have a potential problem. What if they each specify a different class? Or what if no rule is satisfied by $\boldsymbol{X}$?

We tackle the first question. If more than one rule is triggered, we need a **conflict resolution strategy** to figure out which rule gets to fire and assign its class prediction to $\boldsymbol{X}$. There are many possible strategies. We look at two, namely *size ordering* and *rule ordering*.

The **size ordering** scheme assigns the highest priority to the triggering rule that has the "toughest" requirements, where toughness is measured by the rule antecedent *size*. That is, the triggering rule with the most attribute tests is fired.

The **rule ordering** scheme prioritizes the rules beforehand. The ordering may be *class-based* or *rule-based*. With **class-based ordering**, the classes are sorted in order of decreasing "importance" such as by decreasing *order of prevalence*. That is, all the rules for the most prevalent (or most frequent) class come first, the rules for the next prevalent class come next, and so on. Alternatively, they may be sorted based on the misclassification cost per class. Within each class, the rules are not ordered—they don't have to be because they all predict the same class (and so there can be no class conflict!).

With **rule-based ordering**, the rules are organized into one long priority list, according to some measure of rule quality, such as accuracy, coverage, or size (number of attribute tests in the rule antecedent), or based on advice from domain experts. When rule ordering is used, the rule set is known as a **decision list**. With rule ordering, the triggering rule that appears earliest in the list has the highest priority, and so it gets to fire its class prediction. Any other rule that satisfies X is ignored. Most rule-based classification systems use a class-based rule-ordering strategy.

Note that in the first strategy, overall the rules are *unordered*. They can be applied in any order when classifying a tuple. That is, a disjunction (logical OR) is implied between each of the rules. Each rule represents a standalone nugget or piece of knowledge. This is in contrast to the rule ordering (decision list) scheme for which rules must be applied in the prescribed order so as to avoid conflicts. Each rule in a decision list implies the negation of the rules that come before it in the list. Hence, rules in a decision list are more difficult to interpret.

Now that we have seen how we can handle conflicts, let's go back to the scenario where there is no rule satisfied by X. How, then, can we determine the class label of X? In this case, a fallback or **default rule** can be set up to specify a default class, based on a training set. This may be the class in majority or the majority class of the tuples that were not covered by any rule. The default rule is evaluated at the end, if and only if no other rule covers X. The condition in the default rule is empty. In this way, the rule fires when no other rule is satisfied.

In the following sections, we examine how to build a rule-based classifier.

8.4.2 Rule Extraction from a Decision Tree

In Section 8.2, we learned how to build a decision tree classifier from a set of training data. Decision tree classifiers are a popular method of classification—it is easy to understand how decision trees work and they are known for their accuracy. Decision trees can become large and difficult to interpret. In this subsection, we look at how to build a rule-based classifier by extracting IF-THEN rules from a decision tree. In comparison with a decision tree, the IF-THEN rules may be easier for humans to understand, particularly if the decision tree is very large.

To extract rules from a decision tree, one rule is created for each path from the root to a leaf node. Each splitting criterion along a given path is logically ANDed to form the rule antecedent ("IF" part). The leaf node holds the class prediction, forming the rule consequent ("THEN" part).

Example 8.7 **Extracting classification rules from a decision tree.** The decision tree of Figure 8.2 can be converted to classification IF-THEN rules by tracing the path from the root node to each leaf node in the tree. The rules extracted from Figure 8.2 are as follows:

$R1$: IF $age = youth$	AND $student = no$	THEN $buys\_computer = no$
$R2$: IF $age = youth$	AND $student = yes$	THEN $buys\_computer = yes$
$R3$: IF $age = middle\_aged$		THEN $buys\_computer = yes$
$R4$: IF $age = senior$	AND $credit\_rating = excellent$	THEN $buys\_computer = yes$
$R5$: IF $age = senior$	AND $credit\_rating = fair$	THEN $buys\_computer = no$

■

A disjunction (logical OR) is implied between each of the extracted rules. Because the rules are extracted directly from the tree, they are **mutually exclusive** and **exhaustive**. *Mutually exclusive* means that we cannot have rule conflicts here because no two rules will be triggered for the same tuple. (We have one rule per leaf, and any tuple can map to only one leaf.) *Exhaustive* means there is one rule for each possible attribute–value combination, so that this set of rules does not require a default rule. Therefore, the order of the rules does not matter—they are *unordered.*

Since we end up with one rule per leaf, the set of extracted rules is not much simpler than the corresponding decision tree! The extracted rules may be even more difficult to interpret than the original trees in some cases. As an example, Figure 8.7 showed decision trees that suffer from subtree repetition and replication. The resulting set of rules extracted can be large and difficult to follow, because some of the attribute tests may be irrelevant or redundant. So, the plot thickens. Although it is easy to extract rules from a decision tree, we may need to do some more work by pruning the resulting rule set.

"How can we prune the rule set?" For a given rule antecedent, any condition that does not improve the estimated accuracy of the rule can be pruned (i.e., removed), thereby generalizing the rule. C4.5 extracts rules from an unpruned tree, and then prunes the rules using a pessimistic approach similar to its tree pruning method. The training tuples and their associated class labels are used to estimate rule accuracy. However, because this would result in an optimistic estimate, alternatively, the estimate is adjusted to compensate for the bias, resulting in a pessimistic estimate. In addition, any rule that does not contribute to the overall accuracy of the entire rule set can also be pruned.

Other problems arise during rule pruning, however, as the rules *will no longer be* mutually exclusive and exhaustive. For conflict resolution, C4.5 adopts a **class-based ordering scheme**. It groups together all rules for a single class, and then determines a ranking of these class rule sets. Within a rule set, the rules are not ordered. C4.5 orders the class rule sets so as to minimize the number of *false-positive errors* (i.e., where a rule predicts a class, C, but the actual class is not C). The class rule set with the least number of false positives is examined first. Once pruning is complete, a final check is done to remove any duplicates. When choosing a default class, C4.5 does not choose the majority class, because this class will likely have many rules for its tuples. Instead, it selects the class that contains the most training tuples that were not covered by any rule.

8.4.3 Rule Induction Using a Sequential Covering Algorithm

IF-THEN rules can be extracted directly from the training data (i.e., without having to generate a decision tree first) using a **sequential covering algorithm**. The name comes from the notion that the rules are learned *sequentially* (one at a time), where each rule for a given class will ideally *cover* many of the class's tuples (and hopefully none of the tuples of other classes). Sequential covering algorithms are the most widely used approach to mining disjunctive sets of classification rules, and form the topic of this subsection.

There are many sequential covering algorithms. Popular variations include AQ, CN2, and the more recent RIPPER. The general strategy is as follows. Rules are learned one at a time. Each time a rule is learned, the tuples covered by the rule are removed, and the process repeats on the remaining tuples. This sequential learning of rules is in contrast to decision tree induction. Because the path to each leaf in a decision tree corresponds to a rule, we can consider decision tree induction as learning a set of rules *simultaneously*.

A basic sequential covering algorithm is shown in Figure 8.10. Here, rules are learned for one class at a time. Ideally, when learning a rule for a class, C, we would like the rule to cover all (or many) of the training tuples of class C and none (or few) of the tuples

Algorithm: Sequential covering. Learn a set of IF-THEN rules for classification.

Input:

- D, a data set of class-labeled tuples;
- *Att_vals*, the set of all attributes and their possible values.

Output: A set of IF-THEN rules.

Method:

```
(1) Rule_set = {}; // initial set of rules learned is empty
(2) for each class c do
(3)     repeat
(4)         Rule = Learn_One_Rule(D, Att_vals, c);
(5)         remove tuples covered by Rule from D;
(6)         Rule_set = Rule_set + Rule; // add new rule to rule set
(7)     until terminating condition;
(8) endfor
(9) return Rule_Set;
```

Figure 8.10 Basic sequential covering algorithm.

from other classes. In this way, the rules learned should be of high accuracy. The rules need not necessarily be of high coverage. This is because we can have more than one rule for a class, so that different rules may cover different tuples within the same class. The process continues until the terminating condition is met, such as when there are no more training tuples or the quality of a rule returned is below a user-specified threshold. The *Learn_One_Rule* procedure finds the "best" rule for the current class, given the current set of training tuples.

"*How are rules learned?*" Typically, rules are grown in a *general-to-specific* manner (Figure 8.11). We can think of this as a beam search, where we start off with an empty rule and then gradually keep appending attribute tests to it. We append by adding the attribute test as a logical conjunct to the existing condition of the rule antecedent. Suppose our training set, D, consists of loan application data. Attributes regarding each applicant include their age, income, education level, residence, credit rating, and the term of the loan. The classifying attribute is *loan_decision*, which indicates whether a loan is accepted (considered safe) or rejected (considered risky). To learn a rule for the class "accept," we start off with the most general rule possible, that is, the condition of the rule antecedent is empty. The rule is

IF THEN *loan_decision* = *accept*.

We then consider each possible attribute test that may be added to the rule. These can be derived from the parameter *Att_vals*, which contains a list of attributes with their associated values. For example, for an attribute–value pair (*att*, *val*), we can consider attribute tests such as $att = val$, $att \leq val$, $att > val$, and so on. Typically, the training data will contain many attributes, each of which may have several possible values. Finding an optimal rule set becomes computationally explosive. Instead, *Learn_One_Rule*

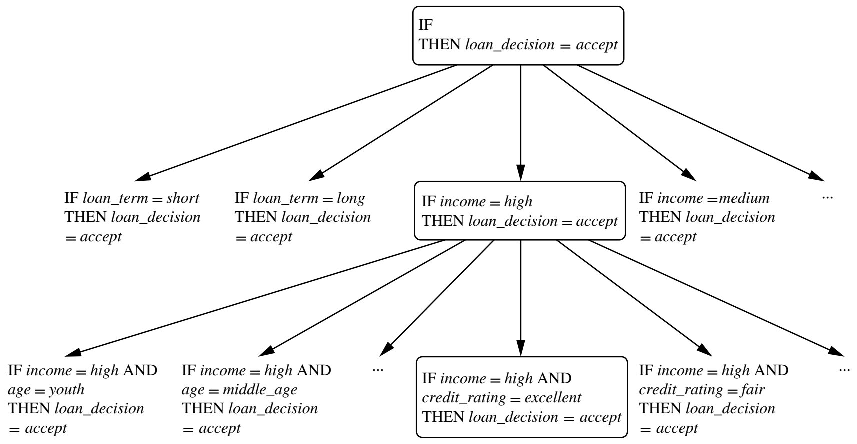

IF THEN loan_decision = accept
IF loan_term = short THEN loan_decision = accept
IF loan_term = long THEN loan_decision = accept
IF income = high THEN loan_decision = accept
IF income = medium THEN loan_decision = accept
...
IF income = high AND age = youth THEN loan_decision = accept
IF income = high AND age = middle_age THEN loan_decision = accept
...
IF income = high AND credit_rating = excellent THEN loan_decision = accept
IF income = high AND credit_rating = fair THEN loan_decision = accept
...

Figure 8.11 A general-to-specific search through rule space.

adopts a greedy depth-first strategy. Each time it is faced with adding a new attribute test (conjunct) to the current rule, it picks the one that most improves the rule quality, based on the training samples. We will say more about rule quality measures in a minute. For the moment, let's say we use rule accuracy as our quality measure. Getting back to our example with Figure 8.11, suppose *Learn_One_Rule* finds that the attribute test *income* = *high* best improves the accuracy of our current (empty) rule. We append it to the condition, so that the current rule becomes

IF *income* = *high* THEN *loan_decision* = *accept*.

Each time we add an attribute test to a rule, the resulting rule should cover relatively more of the "accept" tuples. During the next iteration, we again consider the possible attribute tests and end up selecting *credit_rating* = *excellent*. Our current rule grows to become

IF *income* = *high* AND *credit_rating* = *excellent* THEN *loan_decision* = *accept*.

The process repeats, where at each step we continue to greedily grow rules until the resulting rule meets an acceptable quality level.

Greedy search does not allow for backtracking. At each step, we *heuristically* add what appears to be the best choice at the moment. What if we unknowingly made a poor choice along the way? To lessen the chance of this happening, instead of selecting the best attribute test to append to the current rule, we can select the best *k* attribute tests. In this way, we perform a beam search of width *k*, wherein we maintain the *k* best candidates overall at each step, rather than a single best candidate.

Rule Quality Measures

Learn_One_Rule needs a measure of rule quality. Every time it considers an attribute test, it must check to see if appending such a test to the current rule's condition will result in an improved rule. Accuracy may seem like an obvious choice at first, but consider Example 8.8.

Example 8.8 **Choosing between two rules based on accuracy.** Consider the two rules as illustrated in Figure 8.12. Both are for the class *loan_decision* = *accept*. We use "*a*" to represent the tuples of class "*accept*" and "*r*" for the tuples of class "*reject*." Rule *R*1 correctly classifies 38 of the 40 tuples it covers. Rule *R*2 covers only two tuples, which it correctly classifies. Their respective accuracies are 95% and 100%. Thus, *R*2 has greater accuracy than *R*1, but it is not the better rule because of its small coverage. ■

From this example, we see that accuracy on its own is not a reliable estimate of rule quality. Coverage on its own is not useful either—for a given class we could have a rule that covers many tuples, most of which belong to other classes! Thus, we seek other measures for evaluating rule quality, which may integrate aspects of accuracy and coverage. Here we will look at a few, namely *entropy*, another based on *information gain*, and a *statistical test* that considers coverage. For our discussion, suppose we are learning rules

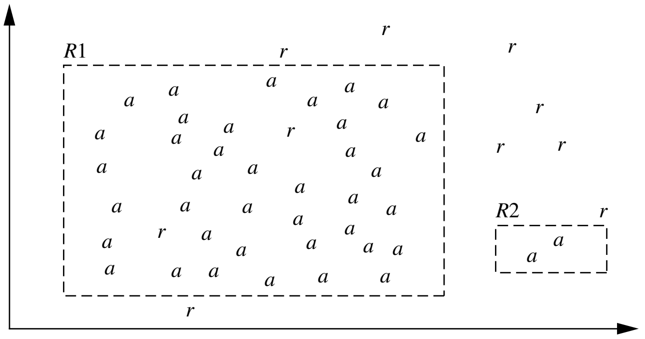


Figure 8.12 Rules for the class *loan_decision* = *accept*, showing *accept* (*a*) and *reject* (*r*) tuples.

for the class *c*. Our current rule is *R*: IF *condition* THEN *class* = *c*. We want to see if logically ANDing a given attribute test to *condition* would result in a better rule. We call the new condition, *condition*′, where *R*′: IF *condition*′ THEN *class* = *c* is our potential new rule. In other words, we want to see if *R*′ is any better than *R*.

We have already seen entropy in our discussion of the information gain measure used for attribute selection in decision tree induction (Section 8.2.2, Eq. 8.1). It is also known as the *expected information* needed to classify a tuple in data set, *D*. Here, *D* is the set of tuples covered by *condition*′ and p_i is the probability of class C_i in *D*. The lower the entropy, the better *condition*′ is. Entropy prefers conditions that cover a large number of tuples of a single class and few tuples of other classes.

Another measure is based on information gain and was proposed in **FOIL** (First Order Inductive Learner), a sequential covering algorithm that learns first-order logic rules. Learning first-order rules is more complex because such rules contain variables, whereas the rules we are concerned with in this section are propositional (i.e., variable-free).[5] In machine learning, the tuples of the class for which we are learning rules are called *positive* tuples, while the remaining tuples are *negative*. Let *pos* (*neg*) be the number of positive (negative) tuples covered by *R*. Let *pos*′ (*neg*′) be the number of positive (negative) tuples covered by *R*′. FOIL assesses the information gained by extending *condition*′ as

$$FOIL\_Gain = pos' \times \left(\log_2 \frac{pos'}{pos' + neg'} - log_2 \frac{pos}{pos + neg}\right). \quad (8.18)$$

It favors rules that have high accuracy and cover many positive tuples.

We can also use a statistical test of significance to determine if the apparent effect of a rule is not attributed to chance but instead indicates a genuine correlation between

[5]Incidentally, FOIL was also proposed by Quinlan, the father of ID3.

attribute values and classes. The test compares the observed distribution among classes of tuples covered by a rule with the expected distribution that would result if the rule made predictions at random. We want to assess whether any observed differences between these two distributions may be attributed to chance. We can use the **likelihood ratio statistic**,

$$Likelihood\_Ratio = 2\sum_{i=1}^{m} f_i \log\left(\frac{f_i}{e_i}\right), \tag{8.19}$$

where m is the number of classes.

For tuples satisfying the rule, f_i is the observed frequency of each class i among the tuples. e_i is what we would expect the frequency of each class i to be if the rule made random predictions. The statistic has a χ^2 distribution with $m-1$ degrees of freedom. The higher the likelihood ratio, the more likely that there is a *significant* difference in the number of correct predictions made by our rule in comparison with a "random guessor." That is, the performance of our rule is not due to chance. The ratio helps identify rules with insignificant coverage.

CN2 uses entropy together with the likelihood ratio test, while FOIL's information gain is used by RIPPER.

Rule Pruning

Learn_One_Rule does not employ a test set when evaluating rules. Assessments of rule quality as described previously are made with tuples from the original training data. These assessments are optimistic because the rules will likely overfit the data. That is, the rules may perform well on the training data, but less well on subsequent data. To compensate for this, we can prune the rules. A rule is pruned by removing a conjunct (attribute test). We choose to prune a rule, R, if the pruned version of R has greater quality, as assessed on an independent set of tuples. As in decision tree pruning, we refer to this set as a *pruning set*. Various pruning strategies can be used such as the pessimistic pruning approach described in the previous section.

FOIL uses a simple yet effective method. Given a rule, R,

$$FOIL\_Prune(R) = \frac{pos - neg}{pos + neg}, \tag{8.20}$$

where pos and neg are the number of positive and negative tuples covered by R, respectively. This value will increase with the accuracy of R on a pruning set. Therefore, if the *FOIL_Prune* value is higher for the pruned version of R, then we prune R.

By convention, RIPPER starts with the most recently added conjunct when considering pruning. Conjuncts are pruned one at a time as long as this results in an improvement.

8.5 Model Evaluation and Selection

Now that you may have built a classification model, there may be many questions going through your mind. For example, suppose you used data from previous sales to build a classifier to predict customer purchasing behavior. You would like an estimate of how accurately the classifier can predict the purchasing behavior of future customers, that is, future customer data on which the classifier has not been trained. You may even have tried different methods to build more than one classifier and now wish to compare their accuracy. But what is accuracy? How can we estimate it? Are some measures of a classifier's accuracy more appropriate than others? How can we obtain a *reliable* accuracy estimate? These questions are addressed in this section.

Section 8.5.1 describes various evaluation metrics for the predictive accuracy of a classifier. Holdout and random subsampling (Section 8.5.2), cross-validation (Section 8.5.3), and bootstrap methods (Section 8.5.4) are common techniques for assessing accuracy, based on randomly sampled partitions of the given data. What if we have more than one classifier and want to choose the "best" one? This is referred to as **model selection** (i.e., choosing one classifier over another). The last two sections address this issue. Section 8.5.5 discusses how to use tests of statistical significance to assess whether the difference in accuracy between two classifiers is due to chance. Section 8.5.6 presents how to compare classifiers based on cost–benefit and receiver operating characteristic (ROC) curves.

8.5.1 Metrics for Evaluating Classifier Performance

This section presents measures for assessing how good or how "accurate" your classifier is at predicting the class label of tuples. We will consider the case of where the class tuples are more or less evenly distributed, as well as the case where classes are unbalanced (e.g., where an important class of interest is rare such as in medical tests). The classifier evaluation measures presented in this section are summarized in Figure 8.13. They include accuracy (also known as recognition rate), sensitivity (or recall), specificity, precision, F_1, and F_β. Note that although accuracy is a specific measure, the word "accuracy" is also used as a general term to refer to a classifier's predictive abilities.

Using training data to derive a classifier and then estimate the accuracy of the resulting learned model can result in misleading overoptimistic estimates due to overspecialization of the learning algorithm to the data. (We will say more on this in a moment!) Instead, it is better to measure the classifier's accuracy on a *test set* consisting of class-labeled tuples that were not used to train the model.

Before we discuss the various measures, we need to become comfortable with some terminology. Recall that we can talk in terms of **positive tuples** (tuples of the main class of interest) and **negative tuples** (all other tuples).[6] Given two classes, for example, the positive tuples may be *buys_computer* = *yes* while the negative tuples are

[6]In the machine learning and pattern recognition literature, these are referred to as *positive samples* and *negative samples*, respectively.

Measure	*Formula*
accuracy, recognition rate	$\frac{TP+TN}{P+N}$
error rate, misclassification rate	$\frac{FP+FN}{P+N}$
sensitivity, true positive rate, recall	$\frac{TP}{P}$
specificity, true negative rate	$\frac{TN}{N}$
precision	$\frac{TP}{TP+FP}$
F, F_1, F-score, harmonic mean of precision and recall	$\frac{2 \times precision \times recall}{precision + recall}$
F_β, where β is a non-negative real number	$\frac{(1+\beta^2) \times precision \times recall}{\beta^2 \times precision + recall}$

Figure 8.13 Evaluation measures. Note that some measures are known by more than one name. TP, TN, FP, P, N refer to the number of true positive, true negative, false positive, positive, and negative samples, respectively (see text).

buys_computer = no. Suppose we use our classifier on a test set of labeled tuples. P is the number of positive tuples and N is the number of negative tuples. For each tuple, we compare the classifier's class label prediction with the tuple's known class label.

There are four additional terms we need to know that are the "building blocks" used in computing many evaluation measures. Understanding them will make it easy to grasp the meaning of the various measures.

- **True positives** (TP): These refer to the positive tuples that were correctly labeled by the classifier. Let TP be the number of true positives.
- **True negatives** (TN): These are the negative tuples that were correctly labeled by the classifier. Let TN be the number of true negatives.
- **False positives** (FP): These are the negative tuples that were incorrectly labeled as positive (e.g., tuples of class *buys_computer = no* for which the classifier predicted *buys_computer = yes*). Let FP be the number of false positives.
- **False negatives** (FN): These are the positive tuples that were mislabeled as negative (e.g., tuples of class *buys_computer = yes* for which the classifier predicted *buys_computer = no*). Let FN be the number of false negatives.

These terms are summarized in the **confusion matrix** of Figure 8.14.

The confusion matrix is a useful tool for analyzing how well your classifier can recognize tuples of different classes. TP and TN tell us when the classifier is getting things right, while FP and FN tell us when the classifier is getting things wrong (i.e.,

		Predicted class		
		yes	*no*	Total
Actual class	*yes*	*TP*	*FN*	*P*
	no	*FP*	*TN*	*N*
	Total	*P′*	*N′*	*P* + *N*

Figure 8.14 Confusion matrix, shown with totals for positive and negative tuples.

Classes	*buys_computer = yes*	*buys_computer = no*	*Total*	*Recognition (%)*
buys_computer = yes	**6954**	**46**	7000	99.34
buys_computer = no	**412**	**2588**	3000	86.27
Total	7366	2634	10,000	95.42

Figure 8.15 Confusion matrix for the classes *buys_computer = yes* and *buys_computer = no,* where an entry in row i and column j shows the number of tuples of class i that were labeled by the classifier as class j. Ideally, the nondiagonal entries should be zero or close to zero.

mislabeling). Given m classes (where $m \geq 2$), a **confusion matrix** is a table of at least size m by m. An entry, $CM_{i,j}$ in the first m rows and m columns indicates the number of tuples of class i that were labeled by the classifier as class j. For a classifier to have good accuracy, ideally most of the tuples would be represented along the diagonal of the confusion matrix, from entry $CM_{1,1}$ to entry $CM_{m,m}$, with the rest of the entries being zero or close to zero. That is, ideally, *FP* and *FN* are around zero.

The table may have additional rows or columns to provide totals. For example, in the confusion matrix of Figure 8.14, P and N are shown. In addition, P' is the number of tuples that were labeled as positive ($TP + FP$) and N' is the number of tuples that were labeled as negative ($TN + FN$). The total number of tuples is $TP + TN + FP + TN$, or $P + N$, or $P' + N'$. Note that although the confusion matrix shown is for a binary classification problem, confusion matrices can be easily drawn for multiple classes in a similar manner.

Now let's look at the evaluation measures, starting with accuracy. The **accuracy** of a classifier on a given test set is the percentage of test set tuples that are correctly classified by the classifier. That is,

$$accuracy = \frac{TP + TN}{P + N}. \tag{8.21}$$

In the pattern recognition literature, this is also referred to as the overall **recognition rate** of the classifier, that is, it reflects how well the classifier recognizes tuples of the various classes. An example of a confusion matrix for the two classes *buys_computer = yes* (positive) and *buys_computer = no* (negative) is given in Figure 8.15. Totals are shown, as well as the recognition rates per class and overall. By glancing at a confusion matrix, it is easy to see if the corresponding classifier is confusing two classes.

For example, we see that it mislabeled 412 *"no"* tuples as *"yes."* Accuracy is most effective when the class distribution is relatively balanced.

We can also speak of the **error rate** or **misclassification rate** of a classifier, M, which is simply $1 - accuracy(M)$, where $accuracy(M)$ is the accuracy of M. This also can be computed as

$$error\ rate = \frac{FP + FN}{P + N}. \tag{8.22}$$

If we were to use the training set (instead of a test set) to estimate the error rate of a model, this quantity is known as the **resubstitution error**. This error estimate is optimistic of the true error rate (and similarly, the corresponding accuracy estimate is optimistic) because the model is not tested on any samples that it has not already seen.

We now consider the **class imbalance problem**, where the main class of interest is rare. That is, the data set distribution reflects a significant majority of the negative class and a minority positive class. For example, in fraud detection applications, the class of interest (or positive class) is *"fraud,"* which occurs much less frequently than the negative *"nonfraudulant"* class. In medical data, there may be a rare class, such as *"cancer."* Suppose that you have trained a classifier to classify medical data tuples, where the class label attribute is *"cancer"* and the possible class values are *"yes"* and *"no."* An accuracy rate of, say, 97% may make the classifier seem quite accurate, but what if only, say, 3% of the training tuples are actually cancer? Clearly, an accuracy rate of 97% may not be acceptable—the classifier could be correctly labeling only the noncancer tuples, for instance, and misclassifying all the cancer tuples. Instead, we need other measures, which access how well the classifier can recognize the positive tuples ($cancer = yes$) and how well it can recognize the negative tuples ($cancer = no$).

The **sensitivity** and **specificity** measures can be used, respectively, for this purpose. Sensitivity is also referred to as the *true positive* (*recognition*) *rate* (i.e., the proportion of positive tuples that are correctly identified), while specificity is the *true negative rate* (i.e., the proportion of negative tuples that are correctly identified). These measures are defined as

$$sensitivity = \frac{TP}{P} \tag{8.23}$$

$$specificity = \frac{TN}{N}. \tag{8.24}$$

It can be shown that accuracy is a function of sensitivity and specificity:

$$accuracy = sensitivity\frac{P}{(P + N)} + specificity\frac{N}{(P + N)}. \tag{8.25}$$

Example 8.9 **Sensitivity and specificity.** Figure 8.16 shows a confusion matrix for medical data where the class values are *yes* and *no* for a class label attribute, *cancer*. The sensitivity

Classes	*yes*	*no*	*Total*	*Recognition (%)*
yes	**90**	**210**	300	30.00
no	**140**	**9560**	9700	98.56
Total	230	9770	10,000	96.40

Figure 8.16 Confusion matrix for the classes *cancer* = *yes* and *cancer* = *no*.

of the classifier is $\frac{90}{300} = 30.00\%$. The specificity is $\frac{9560}{9700} = 98.56\%$. The classifier's overall accuracy is $\frac{9650}{10{,}000} = 96.50\%$. Thus, we note that although the classifier has a high accuracy, it's ability to correctly label the positive (rare) class is poor given its low sensitivity. It has high specificity, meaning that it can accurately recognize negative tuples. Techniques for handling class-imbalanced data are given in Section 8.6.5. ■

The *precision* and *recall* measures are also widely used in classification. **Precision** can be thought of as a measure of *exactness* (i.e., what percentage of tuples labeled as positive are actually such), whereas **recall** is a measure of *completeness* (what percentage of positive tuples are labeled as such). If recall seems familiar, that's because it is the same as sensitivity (or the *true positive rate*). These measures can be computed as

$$precision = \frac{TP}{TP + FP} \tag{8.26}$$

$$recall = \frac{TP}{TP + FN} = \frac{TP}{P}. \tag{8.27}$$

Example 8.10 **Precision and recall.** The precision of the classifier in Figure 8.16 for the *yes* class is $\frac{90}{230} = 39.13\%$. The recall is $\frac{90}{300} = 30.00\%$, which is the same calculation for sensitivity in Example 8.9. ■

A perfect precision score of 1.0 for a class C means that every tuple that the classifier labeled as belonging to class C does indeed belong to class C. However, it does not tell us anything about the number of class C tuples that the classifier mislabeled. A perfect recall score of 1.0 for C means that every item from class C was labeled as such, but it does not tell us how many other tuples were incorrectly labeled as belonging to class C. There tends to be an inverse relationship between precision and recall, where it is possible to increase one at the cost of reducing the other. For example, our medical classifier may achieve high precision by labeling all cancer tuples that present a certain way as *cancer*, but may have low recall if it mislabels many other instances of *cancer* tuples. Precision and recall scores are typically used together, where precision values are compared for a fixed value of recall, or vice versa. For example, we may compare precision values at a recall value of, say, 0.75.

An alternative way to use precision and recall is to combine them into a single measure. This is the approach of the F measure (also known as the F_1 score or F-score) and the F_β measure. They are defined as

$$F = \frac{2 \times precision \times recall}{precision + recall} \tag{8.28}$$

$$F_\beta = \frac{(1+\beta^2) \times precision \times recall}{\beta^2 \times precision + recall}, \tag{8.29}$$

where β is a non-negative real number. The F measure is the *harmonic mean* of precision and recall (the proof of which is left as an exercise). It gives equal weight to precision and recall. The F_β measure is a weighted measure of precision and recall. It assigns β times as much weight to recall as to precision. Commonly used F_β measures are F_2 (which weights recall twice as much as precision) and $F_{0.5}$ (which weights precision twice as much as recall).

"Are there other cases where accuracy may not be appropriate?" In classification problems, it is commonly assumed that all tuples are uniquely classifiable, that is, that each training tuple can belong to only one class. Yet, owing to the wide diversity of data in large databases, it is not always reasonable to assume that all tuples are uniquely classifiable. Rather, it is more probable to assume that each tuple may belong to more than one class. How then can the accuracy of classifiers on large databases be measured? The accuracy measure is not appropriate, because it does not take into account the possibility of tuples belonging to more than one class.

Rather than returning a class label, it is useful to return a probability class distribution. Accuracy measures may then use a **second guess** heuristic, whereby a class prediction is judged as correct if it agrees with the first or second most probable class. Although this does take into consideration, to some degree, the nonunique classification of tuples, it is not a complete solution.

In addition to accuracy-based measures, classifiers can also be compared with respect to the following additional aspects:

- **Speed:** This refers to the computational costs involved in generating and using the given classifier.
- **Robustness:** This is the ability of the classifier to make correct predictions given noisy data or data with missing values. Robustness is typically assessed with a series of synthetic data sets representing increasing degrees of noise and missing values.
- **Scalability:** This refers to the ability to construct the classifier efficiently given large amounts of data. Scalability is typically assessed with a series of data sets of increasing size.
- **Interpretability:** This refers to the level of understanding and insight that is provided by the classifier or predictor. Interpretability is subjective and therefore more difficult to assess. Decision trees and classification rules can be easy to interpret, yet their interpretability may diminish the more they become complex. We discuss some work in this area, such as the extraction of classification rules from a "black box" neural network classifier called backpropagation, in Chapter 9.

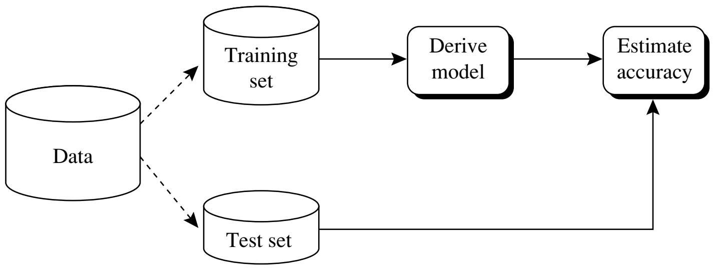


Figure 8.17 Estimating accuracy with the holdout method.

In summary, we have presented several evaluation measures. The accuracy measure works best when the data classes are fairly evenly distributed. Other measures, such as sensitivity (or recall), specificity, precision, F, and F_β, are better suited to the class imbalance problem, where the main class of interest is rare. The remaining subsections focus on obtaining reliable classifier accuracy estimates.

8.5.2 Holdout Method and Random Subsampling

The **holdout** method is what we have alluded to so far in our discussions about accuracy. In this method, the given data are randomly partitioned into two independent sets, a *training set* and a *test set*. Typically, two-thirds of the data are allocated to the training set, and the remaining one-third is allocated to the test set. The training set is used to derive the model. The model's accuracy is then estimated with the test set (Figure 8.17). The estimate is pessimistic because only a portion of the initial data is used to derive the model.

Random subsampling is a variation of the holdout method in which the holdout method is repeated k times. The overall accuracy estimate is taken as the average of the accuracies obtained from each iteration.

8.5.3 Cross-Validation

In ***k*-fold cross-validation**, the initial data are randomly partitioned into k mutually exclusive subsets or "folds," $D_1, D_2, \ldots, D_k$, each of approximately equal size. Training and testing is performed k times. In iteration i, partition D_i is reserved as the test set, and the remaining partitions are collectively used to train the model. That is, in the first iteration, subsets $D_2, \ldots, D_k$ collectively serve as the training set to obtain a first model, which is tested on D_1; the second iteration is trained on subsets $D_1, D_3, \ldots, D_k$ and tested on D_2; and so on. Unlike the holdout and random subsampling methods, here each sample is used the same number of times for training and once for testing. For classification, the accuracy estimate is the overall number of correct classifications from the k iterations, divided by the total number of tuples in the initial data.

Leave-one-out is a special case of k-fold cross-validation where k is set to the number of initial tuples. That is, only one sample is "left out" at a time for the test set. In **stratified cross-validation**, the folds are stratified so that the class distribution of the tuples in each fold is approximately the same as that in the initial data.

In general, stratified 10-fold cross-validation is recommended for estimating accuracy (even if computation power allows using more folds) due to its relatively low bias and variance.

8.5.4 Bootstrap

Unlike the accuracy estimation methods just mentioned, the **bootstrap method** samples the given training tuples uniformly *with replacement*. That is, each time a tuple is selected, it is equally likely to be selected again and re-added to the training set. For instance, imagine a machine that randomly selects tuples for our training set. In *sampling with replacement*, the machine is allowed to select the same tuple more than once.

There are several bootstrap methods. A commonly used one is the **.632 bootstrap**, which works as follows. Suppose we are given a data set of d tuples. The data set is sampled d times, with replacement, resulting in a *bootstrap sample* or training set of d samples. It is very likely that some of the original data tuples will occur more than once in this sample. The data tuples that did not make it into the training set end up forming the test set. Suppose we were to try this out several times. As it turns out, on average, 63.2% of the original data tuples will end up in the bootstrap sample, and the remaining 36.8% will form the test set (hence, the name, .632 bootstrap).

"*Where does the figure, 63.2%, come from?*" Each tuple has a probability of $1/d$ of being selected, so the probability of not being chosen is $(1 - 1/d)$. We have to select d times, so the probability that a tuple will not be chosen during this whole time is $(1 - 1/d)^d$. If d is large, the probability approaches $e^{-1} = 0.368$.[7] Thus, 36.8% of tuples will not be selected for training and thereby end up in the test set, and the remaining 63.2% will form the training set.

We can repeat the sampling procedure k times, where in each iteration, we use the current test set to obtain an accuracy estimate of the model obtained from the current bootstrap sample. The overall accuracy of the model, M, is then estimated as

$$Acc(M) = \frac{1}{k}\sum_{i=1}^{k}(0.632 \times Acc(M_i)_{test\_set} + 0.368 \times Acc(M_i)_{train\_set}), \tag{8.30}$$

where $Acc(M_i)_{test\_set}$ is the accuracy of the model obtained with bootstrap sample i when it is applied to test set i. $Acc(M_i)_{train\_set}$ is the accuracy of the model obtained with bootstrap sample i when it is applied to the original set of data tuples. Bootstrapping tends to be overly optimistic. It works best with small data sets.

[7] e is the base of natural logarithms, that is, $e = 2.718$.

8.5.5 Model Selection Using Statistical Tests of Significance

Suppose that we have generated two classification models, M_1 and M_2, from our data. We have performed 10-fold cross-validation to obtain a mean error rate[8] for each. How can we determine which model is best? It may seem intuitive to select the model with the lowest error rate; however, the mean error rates are just *estimates* of error on the true population of future data cases. There can be considerable variance between error rates within any given 10-fold cross-validation experiment. Although the mean error rates obtained for M_1 and M_2 may appear different, that difference may not be statistically significant. What if any difference between the two may just be attributed to chance? This section addresses these questions.

To determine if there is any "real" difference in the mean error rates of two models, we need to employ a *test of statistical significance*. In addition, we want to obtain some confidence limits for our mean error rates so that we can make statements like, *"Any observed mean will not vary by ± two standard errors 95% of the time for future samples"* or *"One model is better than the other by a margin of error of ± 4%."*

What do we need to perform the statistical test? Suppose that for each model, we did 10-fold cross-validation, say, 10 times, each time using a different 10-fold data partitioning. Each partitioning is independently drawn. We can average the 10 error rates obtained each for M_1 and M_2, respectively, to obtain the mean error rate for each model. For a given model, the individual error rates calculated in the cross-validations may be considered as different, independent samples from a probability distribution. In general, they follow a *t-distribution with* $k-1$ *degrees of freedom* where, here, $k = 10$. (This distribution looks very similar to a normal, or Gaussian, distribution even though the functions defining the two are quite different. Both are unimodal, symmetric, and bell-shaped.) This allows us to do hypothesis testing where the significance test used is the ***t*-test**, or **Student's *t*-test**. Our hypothesis is that the two models are the same, or in other words, that the difference in mean error rate between the two is zero. If we can reject this hypothesis (referred to as the *null hypothesis*), then we can conclude that the difference between the two models is statistically significant, in which case we can select the model with the lower error rate.

In data mining practice, we may often employ a single test set, that is, the same test set can be used for both M_1 and M_2. In such cases, we do a **pairwise comparison** of the two models *for each* 10-fold cross-validation round. That is, for the *i*th round of 10-fold cross-validation, the same cross-validation partitioning is used to obtain an error rate for M_1 and for M_2. Let $err(M_1)_i$ (or $err(M_2)_i$) be the error rate of model M_1 (or M_2) on round i. The error rates for M_1 are averaged to obtain a mean error rate for M_1, denoted $\overline{err}(M_1)$. Similarly, we can obtain $\overline{err}(M_2)$. The variance of the difference between the two models is denoted $var(M_1 - M_2)$. The t-test computes the *t-statistic with* $k-1$ *degrees of freedom* for k samples. In our example we have $k = 10$ since, here, the k samples are our error rates obtained from ten 10-fold cross-validations for each

[8]Recall that the error rate of a model, M, is $1 - accuracy(M)$.

model. The t-statistic for pairwise comparison is computed as follows:

$$t = \frac{\overline{err}(M_1) - \overline{err}(M_2)}{\sqrt{var(M_1 - M_2)/k}}, \tag{8.31}$$

where

$$var(M_1 - M_2) = \frac{1}{k}\sum_{i=1}^{k}\left[err(M_1)_i - err(M_2)_i - (\overline{err}(M_1) - \overline{err}(M_2))\right]^2. \tag{8.32}$$

To determine whether M_1 and M_2 are significantly different, we compute t and select a **significance level**, *sig*. In practice, a significance level of 5% or 1% is typically used. We then consult a table for the *t-distribution*, available in standard textbooks on statistics. This table is usually shown arranged by degrees of freedom as rows and significance levels as columns. Suppose we want to ascertain whether the difference between M_1 and M_2 is significantly different for 95% of the population, that is, $sig = 5\%$ or 0.05. We need to find the t-distribution value corresponding to $k-1$ degrees of freedom (or 9 degrees of freedom for our example) from the table. However, because the t-distribution is symmetric, typically only the upper percentage points of the distribution are shown. Therefore, we look up the table value for $z = sig/2$, which in this case is 0.025, where z is also referred to as a **confidence limit**. If $t > z$ or $t < -z$, then our value of t lies in the rejection region, within the distribution's tails. This means that we can reject the null hypothesis that the means of M_1 and M_2 are the same and conclude that there is a statistically significant difference between the two models. Otherwise, if we cannot reject the null hypothesis, we conclude that any difference between M_1 and M_2 can be attributed to chance.

If two test sets are available instead of a single test set, then a nonpaired version of the t-test is used, where the variance between the means of the two models is estimated as

$$var(M_1 - M_2) = \sqrt{\frac{var(M_1)}{k_1} + \frac{var(M_2)}{k_2}}, \tag{8.33}$$

and k_1 and k_2 are the number of cross-validation samples (in our case, 10-fold cross-validation rounds) used for M_1 and M_2, respectively. This is also known as the **two sample *t*-test**.[9] When consulting the table of t-distribution, the number of degrees of freedom used is taken as the minimum number of degrees of the two models.

8.5.6 Comparing Classifiers Based on Cost–Benefit and ROC Curves

The true positives, true negatives, false positives, and false negatives are also useful in assessing the **costs and benefits** (or risks and gains) associated with a classification

[9]This test was used in sampling cubes for OLAP-based mining in Chapter 5.

model. The cost associated with a false negative (such as incorrectly predicting that a cancerous patient is not cancerous) is far greater than those of a false positive (incorrectly yet conservatively labeling a noncancerous patient as cancerous). In such cases, we can outweigh one type of error over another by assigning a different cost to each. These costs may consider the danger to the patient, financial costs of resulting therapies, and other hospital costs. Similarly, the benefits associated with a true positive decision may be different than those of a true negative. Up to now, to compute classifier accuracy, we have assumed equal costs and essentially divided the sum of true positives and true negatives by the total number of test tuples.

Alternatively, we can incorporate costs and benefits by instead computing the average cost (or benefit) per decision. Other applications involving cost–benefit analysis include loan application decisions and target marketing mailouts. For example, the cost of loaning to a defaulter greatly exceeds that of the lost business incurred by denying a loan to a nondefaulter. Similarly, in an application that tries to identify households that are likely to respond to mailouts of certain promotional material, the cost of mailouts to numerous households that do not respond may outweigh the cost of lost business from not mailing to households that would have responded. Other costs to consider in the overall analysis include the costs to collect the data and to develop the classification tool.

Receiver operating characteristic curves are a useful visual tool for comparing two classification models. ROC curves come from signal detection theory that was developed during World War II for the analysis of radar images. An ROC curve for a given model shows the trade-off between the *true positive rate* (*TPR*) and the *false positive rate* (*FPR*).[10] Given a test set and a model, *TPR* is the proportion of positive (or "yes") tuples that are correctly labeled by the model; *FPR* is the proportion of negative (or "no") tuples that are mislabeled as positive. Given that *TP*, *FP*, *P*, and *N* are the number of true positive, false positive, positive, and negative tuples, respectively, from Section 8.5.1 we know that $TPR = \frac{TP}{P}$, which is sensitivity. Furthermore, $FPR = \frac{FP}{N}$, which is $1 - specificity$.

For a two-class problem, an ROC curve allows us to visualize the trade-off between the rate at which the model can accurately recognize positive cases versus the rate at which it mistakenly identifies negative cases as positive for different portions of the test set. Any increase in *TPR* occurs at the cost of an increase in *FPR*. The area under the ROC curve is a measure of the accuracy of the model.

To plot an ROC curve for a given classification model, *M*, the model must be able to return a probability of the predicted class for each test tuple. With this information, we rank and sort the tuples so that the tuple that is most likely to belong to the positive or "yes" class appears at the top of the list, and the tuple that is least likely to belong to the positive class lands at the bottom of the list. Naïve Bayesian (Section 8.3) and backpropagation (Section 9.2) classifiers return a class probability distribution for each prediction and, therefore, are appropriate, although other classifiers, such as decision tree classifiers (Section 8.2), can easily be modified to return class probability predictions. Let the value

[10] *TPR* and *FPR* are the two operating characteristics being compared.

that a probabilistic classifier returns for a given tuple $\boldsymbol{X}$ be $f(\boldsymbol{X}) \rightarrow [0,1]$. For a binary problem, a threshold t is typically selected so that tuples where $f(\boldsymbol{X}) \geq t$ are considered positive and all the other tuples are considered negative. Note that the number of true positives and the number of false positives are both functions of t, so that we could write $TP(t)$ and $FP(t)$. Both are monotonic descending functions.

We first describe the general idea behind plotting an ROC curve, and then follow up with an example. The vertical axis of an ROC curve represents *TPR*. The horizontal axis represents *FPR*. To plot an ROC curve for *M*, we begin as follows. Starting at the bottom left corner (where $TPR = FPR = 0$), we check the tuple's actual class label at the top of the list. If we have a true positive (i.e., a positive tuple that was correctly classified), then *TP* and thus *TPR* increase. On the graph, we move up and plot a point. If, instead, the model classifies a negative tuple as positive, we have a false positive, and so both *FP* and *FPR* increase. On the graph, we move right and plot a point. This process is repeated for each of the test tuples in ranked order, each time moving up on the graph for a true positive or toward the right for a false positive.

Example 8.11 **Plotting an ROC curve.** Figure 8.18 shows the probability value (column 3) returned by a probabilistic classifier for each of the 10 tuples in a test set, sorted by decreasing probability order. Column 1 is merely a tuple identification number, which aids in our explanation. Column 2 is the actual class label of the tuple. There are five positive tuples and five negative tuples, thus $P = 5$ and $N = 5$. As we examine the known class label of each tuple, we can determine the values of the remaining columns, *TP*, *FP*, *TN*, *FN*, *TPR*, and *FPR*. We start with tuple 1, which has the highest probability score, and take that score as our threshold, that is, $t = 0.9$. Thus, the classifier considers tuple 1 to be positive, and all the other tuples are considered negative. Since the actual class label of tuple 1 is positive, we have a true positive, hence $TP = 1$ and $FP = 0$. Among the

Tuple #	*Class*	*Prob.*	*TP*	*FP*	*TN*	*FN*	*TPR*	*FPR*
1	*P*	0.90	1	0	5	4	0.2	0
2	*P*	0.80	2	0	5	3	0.4	0
3	*N*	0.70	2	1	4	3	0.4	0.2
4	*P*	0.60	3	1	4	2	0.6	0.2
5	*P*	0.55	4	1	4	1	0.8	0.2
6	*N*	0.54	4	2	3	1	0.8	0.4
7	*N*	0.53	4	3	2	1	0.8	0.6
8	*N*	0.51	4	4	1	1	0.8	0.8
9	*P*	0.50	5	4	0	1	1.0	0.8
10	*N*	0.40	5	5	0	0	1.0	1.0

Figure 8.18 Tuples sorted by decreasing score, where the score is the value returned by a probabilistic classifier.

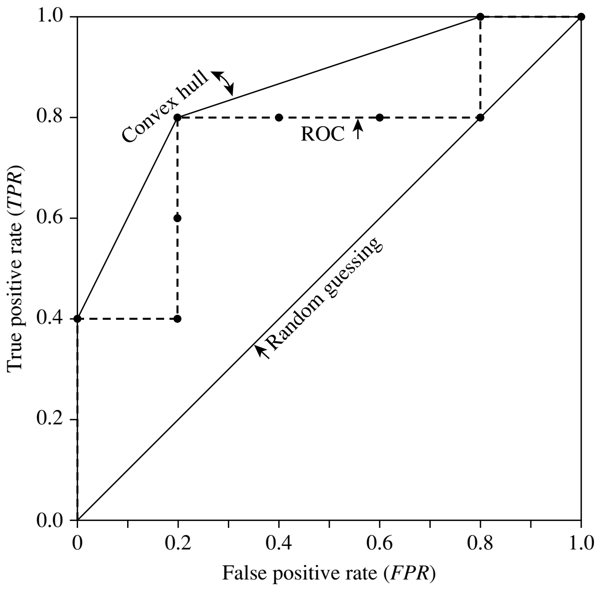


Figure 8.19 ROC curve for the data in Figure 8.18.

remaining nine tuples, which are all classified as negative, five actually are negative (thus, $TN = 5$). The remaining four are all actually positive, thus, $FN = 4$. We can therefore compute $TPR = \frac{TP}{P} = \frac{1}{5} = 0.2$, while $FPR = 0$. Thus, we have the point (0.2,0) for the ROC curve.

Next, threshold t is set to 0.8, the probability value for tuple 2, so this tuple is now also considered positive, while tuples 3 through 10 are considered negative. The actual class label of tuple 2 is positive, thus now $TP = 2$. The rest of the row can easily be computed, resulting in the point (0.4,0). Next, we examine the class label of tuple 3 and let t be 0.7, the probability value returned by the classifier for that tuple. Thus, tuple 3 is considered positive, yet its actual label is negative, and so it is a false positive. Thus, TP stays the same and FP increments so that $FP = 1$. The rest of the values in the row can also be easily computed, yielding the point (0.4,0.2). The resulting ROC graph, from examining each tuple, is the jagged line shown in Figure 8.19.

There are many methods to obtain a curve out of these points, the most common of which is to use a convex hull. The plot also shows a diagonal line where for every true positive of such a model, we are just as likely to encounter a false positive. For comparison, this line represents random guessing. ■

Figure 8.20 shows the ROC curves of two classification models. The diagonal line representing random guessing is also shown. Thus, the closer the ROC curve of a model is to the diagonal line, the less accurate the model. If the model is really good, initially we are more likely to encounter true positives as we move down the ranked list. Thus,

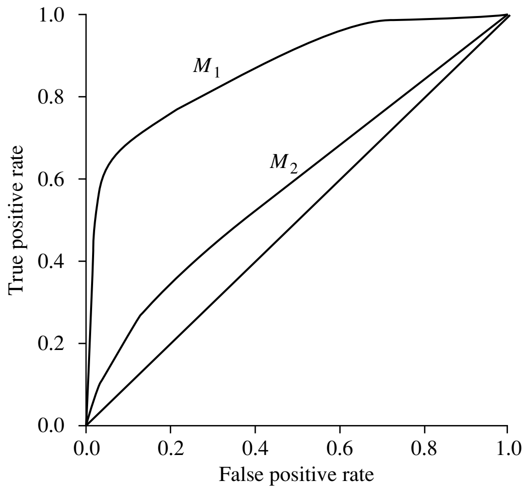


Figure 8.20 ROC curves of two classification models, M_1 and M_2. The diagonal shows where, for every true positive, we are equally likely to encounter a false positive. The closer an ROC curve is to the diagonal line, the less accurate the model is. Thus, $M1$ is more accurate here.

the curve moves steeply up from zero. Later, as we start to encounter fewer and fewer true positives, and more and more false positives, the curve eases off and becomes more horizontal.

To assess the accuracy of a model, we can measure the area under the curve. Several software packages are able to perform such calculation. The closer the area is to 0.5, the less accurate the corresponding model is. A model with perfect accuracy will have an area of 1.0.

8.6 Techniques to Improve Classification Accuracy

In this section, you will learn some tricks for increasing classification accuracy. We focus on *ensemble methods*. An ensemble for classification is a composite model, made up of a combination of classifiers. The individual classifiers vote, and a class label prediction is returned by the ensemble based on the collection of votes. Ensembles tend to be more accurate than their component classifiers. We start off in Section 8.6.1 by introducing ensemble methods in general. Bagging (Section 8.6.2), boosting (Section 8.6.3), and random forests (Section 8.6.4) are popular ensemble methods.

Traditional learning models assume that the data classes are well distributed. In many real-world data domains, however, the data are class-imbalanced, where the main class of interest is represented by only a few tuples. This is known as the *class* *imbalance problem.* We also study techniques for improving the classification accuracy of class-imbalanced data. These are presented in Section 8.6.5.

8.6.1 Introducing Ensemble Methods

Bagging, *boosting*, and *random forests* are examples of **ensemble methods** (Figure 8.21). An ensemble combines a series of k learned models (or *base classifiers*), $M_1, M_2, \ldots, M_k$, with the aim of creating an improved composite classification model, $M*$. A given data set, D, is used to create k training sets, $D_1, D_2, \ldots, D_k$, where D_i $(1 \leq i \leq k-1)$ is used to generate classifier M_i. Given a new data tuple to classify, the base classifiers each vote by returning a class prediction. The ensemble returns a class prediction based on the votes of the base classifiers.

An ensemble tends to be more accurate than its base classifiers. For example, consider an ensemble that performs majority voting. That is, given a tuple $\boldsymbol{X}$ to classify, it collects the class label predictions returned from the base classifiers and outputs the class in majority. The base classifiers may make mistakes, but the ensemble will misclassify $\boldsymbol{X}$ only if over half of the base classifiers are in error. Ensembles yield better results when there is significant diversity among the models. That is, ideally, there is little correlation among classifiers. The classifiers should also perform better than random guessing. Each base classifier can be allocated to a different CPU and so ensemble methods are parallelizable.

To help illustrate the power of an ensemble, consider a simple two-class problem described by two attributes, x_1 and x_2. The problem has a linear decision boundary. Figure 8.22(a) shows the decision boundary of a decision tree classifier on the problem. Figure 8.22(b) shows the decision boundary of an ensemble of decision tree classifiers on the same problem. Although the ensemble's decision boundary is still piecewise constant, it has a finer resolution and is better than that of a single tree.

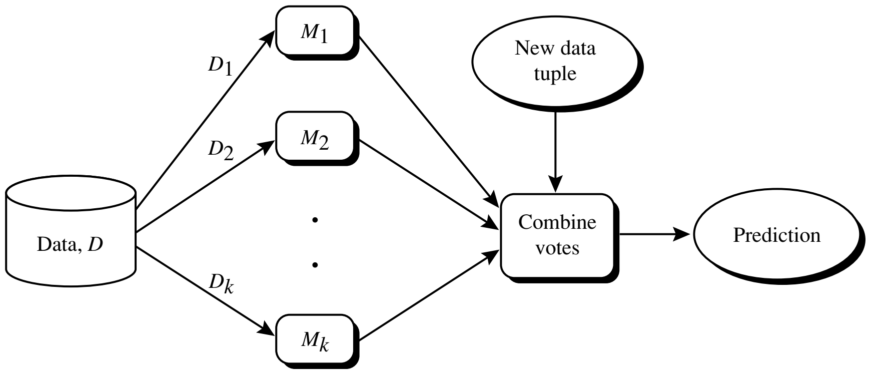


Figure 8.21 Increasing classifier accuracy: Ensemble methods generate a set of classification models, $M_1, M_2, \ldots, M_k$. Given a new data tuple to classify, each classifier "votes" for the class label of that tuple. The ensemble combines the votes to return a class prediction.

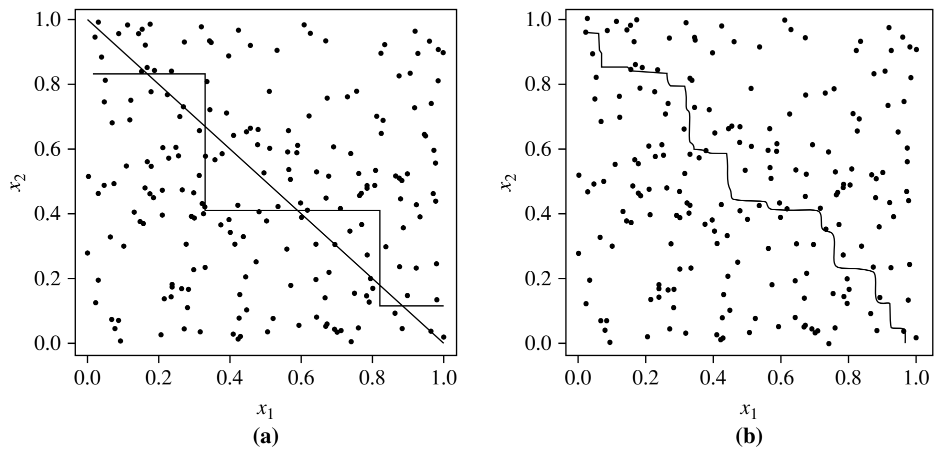


Figure 8.22 Decision boundary by (a) a single decision tree and (b) an ensemble of decision trees for a linearly separable problem (i.e., where the actual decision boundary is a straight line). The decision tree struggles with approximating a linear boundary. The decision boundary of the ensemble is closer to the true boundary. *Source:* From Seni and Elder [SE10]. © 2010 Morgan & Claypool Publishers; used with permission.

8.6.2 Bagging

We now take an intuitive look at how bagging works as a method of increasing accuracy. Suppose that you are a patient and would like to have a diagnosis made based on your symptoms. Instead of asking one doctor, you may choose to ask several. If a certain diagnosis occurs more than any other, you may choose this as the final or best diagnosis. That is, the final diagnosis is made based on a majority vote, where each doctor gets an equal vote. Now replace each doctor by a classifier, and you have the basic idea behind bagging. Intuitively, a majority vote made by a large group of doctors may be more reliable than a majority vote made by a small group.

Given a set, D, of d tuples, **bagging** works as follows. For iteration $i\,(i = 1, 2, \ldots, k)$, a training set, D_i, of d tuples is sampled with replacement from the original set of tuples, D. Note that the term *bagging* stands for *bootstrap aggregation.* Each training set is a bootstrap sample, as described in Section 8.5.4. Because sampling with replacement is used, some of the original tuples of D may not be included in D_i, whereas others may occur more than once. A classifier model, M_i, is learned for each training set, D_i. To classify an unknown tuple, $\boldsymbol{X}$, each classifier, M_i, returns its class prediction, which counts as one vote. The bagged classifier, $M*$, counts the votes and assigns the class with the most votes to $\boldsymbol{X}$. Bagging can be applied to the prediction of continuous values by taking the average value of each prediction for a given test tuple. The algorithm is summarized in Figure 8.23.

The bagged classifier often has significantly greater accuracy than a single classifier derived from D, the original training data. It will not be considerably worse and is more

Algorithm: Bagging. The bagging algorithm—create an ensemble of classification models for a learning scheme where each model gives an equally weighted prediction.

Input:

- D, a set of d training tuples;
- k, the number of models in the ensemble;
- a classification learning scheme (decision tree algorithm, naïve Bayesian, etc.).

Output: The ensemble—a composite model, $M*$.

Method:

```
(1) for $i = 1$ to $k$ do // create $k$ models:
(2)     create bootstrap sample, $D_i$, by sampling $D$ with replacement;
(3)     use $D_i$ and the learning scheme to derive a model, $M_i$;
(4) endfor
```

To use the ensemble to classify a tuple, $\boldsymbol{X}$:

```
    let each of the $k$ models classify $X$ and return the majority vote;
```

Figure 8.23 Bagging.

robust to the effects of noisy data and overfitting. The increased accuracy occurs because the composite model reduces the variance of the individual classifiers.

8.6.3 Boosting and AdaBoost

We now look at the ensemble method of boosting. As in the previous section, suppose that as a patient, you have certain symptoms. Instead of consulting one doctor, you choose to consult several. Suppose you assign weights to the value or worth of each doctor's diagnosis, based on the accuracies of previous diagnoses they have made. The final diagnosis is then a combination of the weighted diagnoses. This is the essence behind boosting.

In **boosting**, weights are also assigned to each training tuple. A series of k classifiers is iteratively learned. After a classifier, M_i, is learned, the weights are updated to allow the subsequent classifier, M_{i+1}, to "pay more attention" to the training tuples that were misclassified by M_i. The final boosted classifier, $M*$, combines the votes of each individual classifier, where the weight of each classifier's vote is a function of its accuracy.

AdaBoost (short for Adaptive Boosting) is a popular boosting algorithm. Suppose we want to boost the accuracy of a learning method. We are given D, a data set of d class-labeled tuples, $(\boldsymbol{X_1}, y_1), (\boldsymbol{X_2}, y_2), \ldots, (\boldsymbol{X_d}, y_d)$, where y_i is the class label of tuple $\boldsymbol{X_i}$. Initially, AdaBoost assigns each training tuple an equal weight of $1/d$. Generating k classifiers for the ensemble requires k rounds through the rest of the algorithm. In round i, the tuples from D are sampled to form a training set, D_i, of size d. Sampling with replacement is used—the same tuple may be selected more than once. Each tuple's chance of being selected is based on its weight. A classifier model, M_i, is derived from the training tuples of D_i. Its error is then calculated using D_i as a test set. The weights of the training tuples are then adjusted according to how they were classified.

If a tuple was incorrectly classified, its weight is increased. If a tuple was correctly classified, its weight is decreased. A tuple's weight reflects how difficult it is to classify—the higher the weight, the more often it has been misclassified. These weights will be used to generate the training samples for the classifier of the next round. The basic idea is that when we build a classifier, we want it to focus more on the misclassified tuples of the previous round. Some classifiers may be better at classifying some "difficult" tuples than others. In this way, we build a series of classifiers that complement each other. The algorithm is summarized in Figure 8.24.

Now, let's look at some of the math that's involved in the algorithm. To compute the error rate of model M_i, we sum the weights of each of the tuples in D_i that M_i misclassified. That is,

$$error(M_i) = \sum_{j=1}^{d} w_j \times err(\boldsymbol{X_j}), \tag{8.34}$$

where $err(\boldsymbol{X_j})$ is the misclassification error of tuple $\boldsymbol{X_j}$: If the tuple was misclassified, then $err(\boldsymbol{X_j})$ is 1; otherwise, it is 0. If the performance of classifier M_i is so poor that its error exceeds 0.5, then we abandon it. Instead, we try again by generating a new D_i training set, from which we derive a new M_i.

The error rate of M_i affects how the weights of the training tuples are updated. If a tuple in round i was correctly classified, its weight is multiplied by $error(M_i)/(1 - error(M_i))$. Once the weights of all the correctly classified tuples are updated, the weights for all tuples (including the misclassified ones) are normalized so that their sum remains the same as it was before. To normalize a weight, we multiply it by the sum of the old weights, divided by the sum of the new weights. As a result, the weights of misclassified tuples are increased and the weights of correctly classified tuples are decreased, as described before.

*"Once boosting is complete, how is the ensemble of classifiers used to predict the class label of a tuple, **X**?"* Unlike bagging, where each classifier was assigned an equal vote, boosting assigns a weight to each classifier's vote, based on how well the classifier performed. The lower a classifier's error rate, the more accurate it is, and therefore, the higher its weight for voting should be. The weight of classifier M_i's vote is

$$log \frac{1 - error(M_i)}{error(M_i)}. \tag{8.35}$$

For each class, c, we sum the weights of each classifier that assigned class c to $\boldsymbol{X}$. The class with the highest sum is the "winner" and is returned as the class prediction for tuple $\boldsymbol{X}$.

"How does boosting compare with bagging?" Because of the way boosting focuses on the misclassified tuples, it risks overfitting the resulting composite model to such data.

Algorithm: AdaBoost. A boosting algorithm—create an ensemble of classifiers. Each one gives a weighted vote.

Input:

- D, a set of d class-labeled training tuples;
- k, the number of rounds (one classifier is generated per round);
- a classification learning scheme.

Output: A composite model.

Method:

```
(1)  initialize the weight of each tuple in $D$ to $1/d$;
(2)  for $i = 1$ to $k$ do // for each round:
(3)      sample $D$ with replacement according to the tuple weights to obtain $D_i$;
(4)      use training set $D_i$ to derive a model, $M_i$;
(5)      compute $error(M_i)$, the error rate of $M_i$ (Eq. 8.34)
(6)      if $error(M_i) > 0.5$ then
(7)          go back to step 3 and try again;
(8)      endif
(9)      for each tuple in $D_i$ that was correctly classified do
(10)         multiply the weight of the tuple by $error(M_i)/(1 - error(M_i))$; // update weights
(11)     normalize the weight of each tuple;
(12) endfor
```

To use the ensemble to classify tuple, X:

```
(1)  initialize weight of each class to 0;
(2)  for $i = 1$ to $k$ do // for each classifier:
(3)      $w_i = log\frac{1-error(M_i)}{error(M_i)}$; // weight of the classifier's vote
(4)      $c = M_i(X)$; // get class prediction for $X$ from $M_i$
(5)      add $w_i$ to weight for class $c$
(6)  endfor
(7)  return the class with the largest weight;
```

Figure 8.24 AdaBoost, a boosting algorithm.

Therefore, sometimes the resulting "boosted" model may be less accurate than a single model derived from the same data. Bagging is less susceptible to model overfitting. While both can significantly improve accuracy in comparison to a single model, boosting tends to achieve greater accuracy.

8.6.4 Random Forests

We now present another ensemble method called **random forests**. Imagine that each of the classifiers in the ensemble is a *decision tree* classifier so that the collection of classifiers is a “forest.” The individual decision trees are generated using a random selection of attributes at each node to determine the split. More formally, each tree depends on the values of a random vector sampled independently and with the same distribution for all trees in the forest. During classification, each tree votes and the most popular class is returned.

Random forests can be built using bagging (Section 8.6.2) in tandem with random attribute selection. A training set, D, of d tuples is given. The general procedure to generate k decision trees for the ensemble is as follows. For each iteration, $i (i = 1, 2, \ldots, k)$, a training set, D_i, of d tuples is sampled with replacement from D. That is, each D_i is a bootstrap sample of D (Section 8.5.4), so that some tuples may occur more than once in D_i, while others may be excluded. Let F be the number of attributes to be used to determine the split at each node, where F is much smaller than the number of available attributes. To construct a decision tree classifier, M_i, randomly select, at each node, F attributes as candidates for the split at the node. The CART methodology is used to grow the trees. The trees are grown to maximum size and are not pruned. Random forests formed this way, with *random input selection*, are called Forest-RI.

Another form of random forest, called Forest-RC, uses *random linear combinations* of the input attributes. Instead of randomly selecting a subset of the attributes, it creates new attributes (or features) that are a linear combination of the existing attributes. That is, an attribute is generated by specifying L, the number of original attributes to be combined. At a given node, L attributes are randomly selected and added together with coefficients that are uniform random numbers on $[-1, 1]$. F linear combinations are generated, and a search is made over these for the best split. This form of random forest is useful when there are only a few attributes available, so as to reduce the correlation between individual classifiers.

Random forests are comparable in accuracy to AdaBoost, yet are more robust to errors and outliers. The generalization error for a forest converges as long as the number of trees in the forest is large. Thus, overfitting is not a problem. The accuracy of a random forest depends on the strength of the individual classifiers and a measure of the dependence between them. The ideal is to maintain the strength of individual classifiers without increasing their correlation. Random forests are insensitive to the number of attributes selected for consideration at each split. Typically, up to $log_2 d + 1$ are chosen. (An interesting empirical observation was that using a single random input attribute may result in good accuracy that is often higher than when using several attributes.) Because random forests consider many fewer attributes for each split, they are efficient on very large databases. They can be faster than either bagging or boosting. Random forests give internal estimates of variable importance.

8.6.5 Improving Classification Accuracy of Class-Imbalanced Data

In this section, we revisit the *class imbalance problem*. In particular, we study approaches to improving the classification accuracy of class-imbalanced data.

Given two-class data, the data are class-imbalanced if the main class of interest (the positive class) is represented by only a few tuples, while the majority of tuples represent the negative class. For multiclass-imbalanced data, the data distribution of each class differs substantially where, again, the main class or classes of interest are rare. The class imbalance problem is closely related to cost-sensitive learning, wherein the costs of errors, per class, are not equal. In medical diagnosis, for example, it is much more costly to falsely diagnose a cancerous patient as healthy (a false negative) than to misdiagnose a healthy patient as having cancer (a false positive). A false negative error could lead to the loss of life and therefore is much more expensive than a false positive error. Other applications involving class-imbalanced data include fraud detection, the detection of oil spills from satellite radar images, and fault monitoring.

Traditional classification algorithms aim to minimize the number of errors made during classification. They assume that the costs of false positive and false negative errors are equal. By assuming a balanced distribution of classes and equal error costs, they are therefore not suitable for class-imbalanced data. Earlier parts of this chapter presented ways of addressing the class imbalance problem. Although the accuracy measure assumes that the cost of classes are equal, alternative evaluation metrics can be used that consider the different types of classifications. Section 8.5.1, for example, presented *sensitivity* or recall (the true positive rate) and *specificity* (the true negative rate), which help to assess how well a classifier can predict the class label of imbalanced data. Additional relevant measures discussed include F_1 and F_β. Section 8.5.6 showed how ROC curves plot *sensitivity* versus 1 − *specificity* (i.e., the false positive rate). Such curves can provide insight when studying the performance of classifiers on class-imbalanced data.

In this section, we look at general approaches for *improving* the classification accuracy of class-imbalanced data. These approaches include (1) oversampling, (2) undersampling, (3) threshold moving, and (4) ensemble techniques. The first three do not involve any changes to the construction of the classification model. That is, oversampling and undersampling change the distribution of tuples in the training set; threshold moving affects how the model makes decisions when classifying new data. Ensemble methods follow the techniques described in Sections 8.6.2 through 8.6.4. For ease of explanation, we describe these general approaches with respect to the two-class imbalance data problem, where the higher-cost classes are rarer than the lower-cost classes.

Both oversampling and undersampling change the training data distribution so that the rare (positive) class is well represented. **Oversampling** works by resampling the positive tuples so that the resulting training set contains an equal number of positive and negative tuples. **Undersampling** works by decreasing the number of negative tuples. It randomly eliminates tuples from the majority (negative) class until there are an equal number of positive and negative tuples.

Example 8.12 **Oversampling and undersampling.** Suppose the original training set contains 100 positive and 1000 negative tuples. In oversampling, we replicate tuples of the rarer class to form a new training set containing 1000 positive tuples and 1000 negative tuples. In undersampling, we randomly eliminate negative tuples so that the new training set contains 100 positive tuples and 100 negative tuples. ■

Several variations to oversampling and undersampling exist. They may vary, for instance, in how tuples are added or eliminated. For example, the SMOTE algorithm uses oversampling where synthetic tuples are added, which are "close to" the given positive tuples in tuple space.

The **threshold-moving** approach to the class imbalance problem does not involve any sampling. It applies to classifiers that, given an input tuple, return a continuous output value (just like in Section 8.5.6, where we discussed how to construct ROC curves). That is, for an input tuple, $\boldsymbol{X}$, such a classifier returns as output a mapping, $f(\boldsymbol{X}) \rightarrow [0,1]$. Rather than manipulating the training tuples, this method returns a classification decision based on the output values. In the simplest approach, tuples for which $f(\boldsymbol{X}) \geq t$, for some threshold, t, are considered positive, while all other tuples are considered negative. Other approaches may involve manipulating the outputs by weighting. In general, threshold moving moves the threshold, t, so that the rare class tuples are easier to classify (and hence, there is less chance of costly false negative errors). Examples of such classifiers include naïve Bayesian classifiers (Section 8.3) and neural network classifiers like backpropagation (Section 9.2). The threshold-moving method, although not as popular as over- and undersampling, is simple and has shown some success for the two-class-imbalanced data.

Ensemble methods (Sections 8.6.2 through 8.6.4) have also been applied to the class imbalance problem. The individual classifiers making up the ensemble may include versions of the approaches described here such as oversampling and threshold moving.

These methods work relatively well for the class imbalance problem on two-class tasks. Threshold-moving and ensemble methods were empirically observed to outperform oversampling and undersampling. Threshold moving works well even on data sets that are extremely imbalanced. The class imbalance problem on multiclass tasks is much more difficult, where oversampling and threshold moving are less effective. Although threshold-moving and ensemble methods show promise, finding a solution for the multiclass imbalance problem remains an area of future work.

8.7 Summary

- **Classification** is a form of data analysis that extracts models describing data classes. A classifier, or classification model, predicts categorical labels (classes). **Numeric prediction** models continuous-valued functions. Classification and numeric prediction are the two major types of prediction problems.

- **Decision tree induction** is a top-down recursive tree induction algorithm, which uses an attribute selection measure to select the attribute tested for each nonleaf node in the tree. **ID3**, **C4.5**, and **CART** are examples of such algorithms using different attribute selection measures. **Tree pruning** algorithms attempt to improve accuracy by removing tree branches reflecting noise in the data. Early decision tree algorithms typically assume that the data are memory resident. Several scalable algorithms, such as **RainForest**, have been proposed for scalable tree induction.

- **Naïve Bayesian classification** is based on Bayes' theorem of posterior probability. It assumes class-conditional independence—that the effect of an attribute value on a given class is independent of the values of the other attributes.

- A **rule-based classifier** uses a set of IF-THEN rules for classification. Rules can be extracted from a decision tree. Rules may also be generated directly from training data using sequential covering algorithms.
- A **confusion matrix** can be used to evaluate a classifier's quality. For a two-class problem, it shows the *true positives, true negatives, false positives*, and *false negatives.* Measures that assess a classifier's predictive ability include **accuracy**, **sensitivity** (also known as **recall**), **specificity**, **precision**, F, and F_β. Reliance on the accuracy measure can be deceiving when the main class of interest is in the minority.
- Construction and evaluation of a classifier require partitioning labeled data into a training set and a test set. **Holdout, random sampling, cross-validation**, and **bootstrapping** are typical methods used for such partitioning.
- Significance tests and ROC curves are useful tools for model selection. **Significance tests** can be used to assess whether the difference in accuracy between two classifiers is due to chance. **ROC curves** plot the true positive rate (or sensitivity) versus the false positive rate (or $1 -$ *specificity*) of one or more classifiers.
- **Ensemble methods** can be used to increase overall accuracy by learning and combining a series of individual (base) classifier models. **Bagging, boosting**, and **random forests** are popular ensemble methods.
- The **class imbalance problem** occurs when the main class of interest is represented by only a few tuples. Strategies to address this problem include **oversampling, undersampling, threshold moving,** and **ensemble techniques**.

8.8 Exercises

8.1 Briefly outline the major steps of *decision tree classification.*

8.2 Why is *tree pruning* useful in decision tree induction? What is a drawback of using a separate set of tuples to evaluate pruning?

8.3 Given a decision tree, you have the option of (a) *converting* the decision tree to rules and then pruning the resulting rules, or (b) *pruning* the decision tree and then converting the pruned tree to rules. What advantage does (a) have over (b)?

8.4 It is important to calculate the worst-case computational complexity of the decision tree algorithm. Given data set, D, the number of attributes, n, and the number of training tuples, $|D|$, show that the computational cost of growing a tree is at most $n \times |D| \times log(|D|)$.

8.5 Given a 5-GB data set with 50 attributes (each containing 100 distinct values) and 512 MB of main memory in your laptop, outline an efficient method that constructs decision trees in such large data sets. Justify your answer by rough calculation of your main memory usage.

8.6 Why is *naïve Bayesian classification* called "naïve"? Briefly outline the major ideas of naïve Bayesian classification.

8.7 The following table consists of training data from an employee database. The data have been generalized. For example, "31 ... 35" for *age* represents the age range of 31 to 35. For a given row entry, *count* represents the number of data tuples having the values for *department, status, age*, and *salary* given in that row.

department	*status*	*age*	*salary*	*count*
sales	senior	31...35	46K...50K	30
sales	junior	26...30	26K...30K	40
sales	junior	31...35	31K...35K	40
systems	junior	21...25	46K...50K	20
systems	senior	31...35	66K...70K	5
systems	junior	26...30	46K...50K	3
systems	senior	41...45	66K...70K	3
marketing	senior	36...40	46K...50K	10
marketing	junior	31...35	41K...45K	4
secretary	senior	46...50	36K...40K	4
secretary	junior	26...30	26K...30K	6

Let *status* be the class label attribute.

(a) How would you modify the basic decision tree algorithm to take into consideration the *count* of each generalized data tuple (i.e., of each row entry)?

(b) Use your algorithm to construct a decision tree from the given data.

(c) Given a data tuple having the values *"systems," "26...30,"* and *"46–50K"* for the attributes *department, age*, and *salary*, respectively, what would a naïve Bayesian classification of the *status* for the tuple be?

8.8 RainForest is a scalable algorithm for decision tree induction. Develop a scalable naïve Bayesian classification algorithm that requires just a single scan of the entire data set for most databases. Discuss whether such an algorithm can be refined to incorporate *boosting* to further enhance its classification accuracy.

8.9 Design an efficient method that performs effective naïve Bayesian classification over an *infinite* data stream (i.e., you can scan the data stream only once). If we wanted to discover the *evolution* of such classification schemes (e.g., comparing the classification scheme at this moment with earlier schemes such as one from a week ago), what modified design would you suggest?

8.10 Show that accuracy is a function of *sensitivity* and *specificity*, that is, prove Eq. (8.25).

8.11 The harmonic mean is one of several kinds of averages. Chapter 2 discussed how to compute the *arithmetic mean*, which is what most people typically think of when they compute an average. The **harmonic mean**, H, of the positive real numbers, $x_1, x_2, \ldots, x_n$, is defined as

$$H = \frac{n}{\frac{1}{x_1} + \frac{1}{x_2} + \cdots + \frac{1}{x_n}}$$
$$= \frac{n}{\sum_{i=1}^{n} \frac{1}{x_i}}.$$

The F measure is the harmonic mean of precision and recall. Use this fact to derive Eq. (8.28) for F. In addition, write F_β as a function of true positives, false negatives, and false positives.

8.12 The data tuples of Figure 8.25 are sorted by decreasing probability value, as returned by a classifier. For each tuple, compute the values for the number of true positives (TP), false positives (FP), true negatives (TN), and false negatives (FN). Compute the true positive rate (TPR) and false positive rate (FPR). Plot the ROC curve for the data.

8.13 It is difficult to assess classification *accuracy* when individual data objects may belong to more than one class at a time. In such cases, comment on what criteria you would use to compare different classifiers modeled after the same data.

8.14 Suppose that we want to *select between two prediction models*, M_1 and M_2. We have performed 10 rounds of 10-fold cross-validation on each model, where the same data partitioning in round i is used for both M_1 and M_2. The error rates obtained for M_1 are 30.5, 32.2, 20.7, 20.6, 31.0, 41.0, 27.7, 26.0, 21.5, 26.0. The error rates for M_2 are 22.4, 14.5, 22.4, 19.6, 20.7, 20.4, 22.1, 19.4, 16.2, 35.0. Comment on whether one model is significantly better than the other considering a significance level of 1%.

8.15 What is *boosting*? State why it may improve the accuracy of decision tree induction.

Tuple #	*Class*	*Probability*
1	P	0.95
2	N	0.85
3	P	0.78
4	P	0.66
5	N	0.60
6	P	0.55
7	N	0.53
8	N	0.52
9	N	0.51
10	P	0.40

Figure 8.25 Tuples sorted by decreasing score, where the score is the value returned by a probabilistic classifier.

8.16 Outline methods for addressing the *class imbalance problem.* Suppose a bank wants to develop a classifier that guards against fraudulent credit card transactions. Illustrate how you can induce a quality classifier based on a large set of nonfraudulent examples and a very small set of fraudulent cases.

8.9 Bibliographic Notes

Classification is a fundamental topic in machine learning, statistics, and pattern recognition. Many textbooks from these fields highlight classification methods such as Mitchell [Mit97]; Bishop [Bis06]; Duda, Hart, and Stork [DHS01]; Theodoridis and Koutroumbas [TK08]; Hastie, Tibshirani, and Friedman [HTF09]; Alpaydin [Alp11]; and Marsland [Mar09].

For decision tree induction, the C4.5 algorithm is described in a book by Quinlan [Qui93]. The CART system is detailed in *Classification and Regression Trees* by Breiman, Friedman, Olshen, and Stone [BFOS84]. Both books give an excellent presentation of many of the issues regarding decision tree induction. C4.5 has a commercial successor, known as C5.0, which can be found at *www.rulequest.com.* ID3, a predecessor of C4.5, is detailed in Quinlan [Qui86]. It expands on pioneering work on concept learning systems, described by Hunt, Marin, and Stone [HMS66].

Other algorithms for decision tree induction include FACT (Loh and Vanichsetakul [LV88]), QUEST (Loh and Shih [LS97]), PUBLIC (Rastogi and Shim [RS98]), and CHAID (Kass [Kas80] and Magidson [Mag94]). INFERULE (Uthurusamy, Fayyad, and Spangler [UFS91]) learns decision trees from inconclusive data, where probabilistic rather than categorical classification rules are obtained. KATE (Manago and Kodratoff [MK91]) learns decision trees from complex structured data. Incremental versions of ID3 include ID4 (Schlimmer and Fisher [SF86]) and ID5 (Utgoff [Utg88]), the latter of which is extended in Utgoff, Berkman, and Clouse [UBC97]. An incremental version of CART is described in Crawford [Cra89]. BOAT (Gehrke, Ganti, Ramakrishnan, and Loh [GGRL99]), a decision tree algorithm that addresses the scalability issue in data mining, is also incremental. Other decision tree algorithms that address scalability include SLIQ (Mehta, Agrawal, and Rissanen [MAR96]), SPRINT (Shafer, Agrawal, and Mehta [SAM96]), RainForest (Gehrke, Ramakrishnan, and Ganti [GRG98]), and earlier approaches such as Catlet [Cat91] and Chan and Stolfo [CS93a, CS93b].

For a comprehensive survey of many salient issues relating to decision tree induction, such as attribute selection and pruning, see Murthy [Mur98]. Perception-based classification (PBC), a visual and interactive approach to decision tree construction, is presented in Ankerst, Elsen, Ester, and Kriegel [AEEK99].

For a detailed discussion on attribute selection measures, see Kononenko and Hong [KH97]. Information gain was proposed by Quinlan [Qui86] and is based on pioneering work on information theory by Shannon and Weaver [SW49]. The gain ratio, proposed as an extension to information gain, is described as part of C4.5 (Quinlan [Qui93]). The Gini index was proposed for CART in Breiman, Friedman, Olshen, and

Stone [BFOS84]. The G-statistic, based on information theory, is given in Sokal and Rohlf [SR81]. Comparisons of attribute selection measures include Buntine and Niblett [BN92], Fayyad and Irani [FI92], Kononenko [Kon95], Loh and Shih [LS97], and Shih [Shi99]. Fayyad and Irani [FI92] show limitations of impurity-based measures such as information gain and the Gini index. They propose a class of attribute selection measures called C-SEP (Class SEParation), which outperform impurity-based measures in certain cases.

Kononenko [Kon95] notes that attribute selection measures based on the minimum description length principle have the least bias toward multivalued attributes. Martin and Hirschberg [MH95] proved that the time complexity of decision tree induction increases exponentially with respect to tree height in the worst case, and under fairly general conditions in the average case. Fayad and Irani [FI90] found that shallow decision trees tend to have many leaves and higher error rates for a large variety of domains. Attribute (or feature) construction is described in Liu and Motoda [LM98a, LM98b].

There are numerous algorithms for decision tree pruning, including cost complexity pruning (Breiman, Friedman, Olshen, and Stone [BFOS84]), reduced error pruning (Quinlan [Qui87]), and pessimistic pruning (Quinlan [Qui86]). PUBLIC (Rastogi and Shim [RS98]) integrates decision tree construction with tree pruning. MDL-based pruning methods can be found in Quinlan and Rivest [QR89]; Mehta, Agrawal, and Rissanen [MAR96]; and Rastogi and Shim [RS98]. Other methods include Niblett and Bratko [NB86] and Hosking, Pednault, and Sudan [HPS97]. For an empirical comparison of pruning methods, see Mingers [Min89] and Malerba, Floriana, and Semeraro [MFS95]. For a survey on simplifying decision trees, see Breslow and Aha [BA97].

Thorough presentations of Bayesian classification can be found in Duda, Hart, and Stork [DHS01], Weiss and Kulikowski [WK91], and Mitchell [Mit97]. For an analysis of the predictive power of naïve Bayesian classifiers when the class-conditional independence assumption is violated, see Domingos and Pazzani [DP96]. Experiments with kernel density estimation for continuous-valued attributes, rather than Gaussian estimation, have been reported for naïve Bayesian classifiers in John [Joh97].

There are several examples of rule-based classifiers. These include AQ15 (Hong, Mozetic, and Michalski [HMM86]), CN2 (Clark and Niblett [CN89]), ITRULE (Smyth and Goodman [SG92]), RISE (Domingos [Dom94]), IREP (Furnkranz and Widmer [FW94]), RIPPER (Cohen [Coh95]), FOIL (Quinlan and Cameron-Jones [Qui90, QC-J93]), and Swap-1 (Weiss and Indurkhya [WI98]). Rule-based classifiers that are based on frequent-pattern mining are described in Chapter 9. For the extraction of rules from decision trees, see Quinlan [Qui87, Qui93]. Rule refinement strategies that identify the most interesting rules among a given rule set can be found in Major and Mangano [MM95].

Issues involved in estimating classifier accuracy are described in Weiss and Kulikowski [WK91] and Witten and Frank [WF05]. Sensitivity, specificity, and precision are discussed in most information retrieval textbooks. For the F and F_β measures, see van Rijsbergen [vR90]. The use of stratified 10-fold cross-validation for estimating classifier accuracy is recommended over the holdout, cross-validation, leave-one-out (Stone [Sto74]), and bootstrapping (Efron and Tibshirani [ET93]) methods, based on a theoretical and empirical study by Kohavi [Koh95]. See Freedman, Pisani, and Purves [FPP07] for the confidence limits and statistical tests of significance.

For ROC analysis, see Egan [Ega75], Swets [Swe88], and Vuk and Curk [VC06]. Bagging is proposed in Breiman [Bre96]. Freund and Schapire [FS97] proposed AdaBoost. This boosting technique has been applied to several different classifiers, including decision tree induction (Quinlan [Qui96]) and naïve Bayesian classification (Elkan [Elk97]). Friedman [Fri01] proposed the gradient boosting machine for regression. The ensemble technique of random forests is described by Breiman [Bre01]. Seni and Elder [SE10] proposed the Importance Sampling Learning Ensembles (ISLE) framework, which views bagging, AdaBoost, random forests, and gradient boosting as special cases of a generic ensemble generation procedure.

Friedman and Popescu [FB08, FP05] present Rule Ensembles, an ISLE-based model where the classifiers combined are composed of simple readable rules. Such ensembles were observed to have comparable or greater accuracy and greater interpretability. There are many online software packages for ensemble routines, including bagging, AdaBoost, gradient boosting, and random forests. Studies on the class imbalance problem and/or cost-sensitive learning include Weiss [Wei04], Zhou and Liu [ZL06], Zapkowicz and Stephen [ZS02], Elkan [Elk01], and Domingos [Dom99].

The University of California at Irvine (UCI) maintains a Machine Learning Repository of data sets for the development and testing of classification algorithms. It also maintains a Knowledge Discovery in Databases (KDD) Archive, an online repository of large data sets that encompasses a wide variety of data types, analysis tasks, and application areas. For information on these two repositories, see *www.ics.uci.edu/∼mlearn/MLRepository.html* and *http://kdd.ics.uci.edu.*

No classification method is superior to all others for all data types and domains. Empirical comparisons of classification methods include Quinlan [Qui88]; Shavlik, Mooney, and Towell [SMT91]; Brown, Corruble, and Pittard [BCP93]; Curram and Mingers [CM94]; Michie, Spiegelhalter, and Taylor [MST94]; Brodley and Utgoff [BU95]; and Lim, Loh, and Shih [LLS00].

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9 Classification: Advanced Methods

In this chapter, you will learn advanced techniques for data classification. We start with **Bayesian belief networks** (Section 9.1), which unlike naïve Bayesian classifiers, do not assume class conditional independence. **Backpropagation**, a neural network algorithm, is discussed in Section 9.2. In general terms, a neural network is a set of connected input/output units in which each connection has a weight associated with it. The weights are adjusted during the learning phase to help the network predict the correct class label of the input tuples. A more recent approach to classification known as support vector machines is presented in Section 9.3. A **support vector machine** transforms training data into a higher dimension, where it finds a hyperplane that separates the data by class using essential training tuples called *support vectors*. Section 9.4 describes **classification using frequent patterns**, exploring relationships between attribute–value pairs that occur frequently in data. This methodology builds on research on frequent pattern mining (Chapters 6 and 7).

Section 9.5 presents **lazy learners** or **instance-based** methods of classification, such as nearest-neighbor classifiers and case-based reasoning classifiers, which store all of the training tuples in pattern space and wait until presented with a test tuple before performing generalization. Other approaches to classification, such as genetic algorithms, rough sets, and fuzzy logic techniques, are introduced in Section 9.6. Section 9.7 introduces additional topics in classification, including multiclass classification, semi-supervised classification, active learning, and transfer learning.

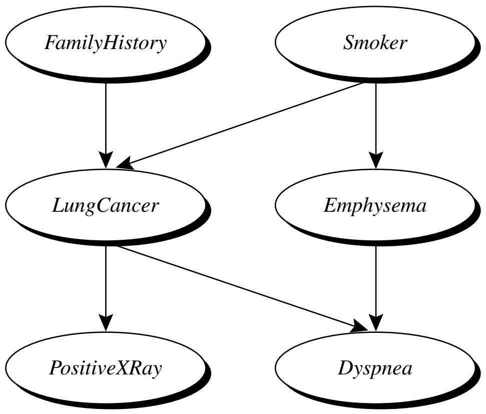
9.1 Bayesian Belief Networks

Chapter 8 introduced Bayes' theorem and naïve Bayesian classification. In this chapter, we describe *Bayesian belief networks*—probabilistic graphical models, which unlike naïve Bayesian classifiers allow the representation of dependencies among subsets of attributes. Bayesian belief networks can be used for classification. Section 9.1.1 introduces the basic concepts of Bayesian belief networks. In Section 9.1.2, you will learn how to train such models.

9.1.1 Concepts and Mechanisms

The naïve Bayesian classifier makes the assumption of class conditional independence, that is, given the class label of a tuple, the values of the attributes are assumed to be conditionally independent of one another. This simplifies computation. When the assumption holds true, then the naïve Bayesian classifier is the most accurate in comparison with all other classifiers. In practice, however, dependencies can exist between variables. **Bayesian belief networks** specify joint conditional probability distributions. They allow class conditional independencies to be defined between subsets of variables. They provide a graphical model of causal relationships, on which learning can be performed. Trained Bayesian belief networks can be used for classification. Bayesian belief networks are also known as **belief networks**, **Bayesian networks**, and **probabilistic networks**. For brevity, we will refer to them as belief networks.

A belief network is defined by two components—a *directed acyclic graph* and a set of *conditional probability tables* (Figure 9.1). Each node in the directed acyclic graph represents a random variable. The variables may be discrete- or continuous-valued. They may correspond to actual attributes given in the data or to "hidden variables" believed to form a relationship (e.g., in the case of medical data, a hidden variable may indicate a syndrome, representing a number of symptoms that, together, characterize a specific disease). Each arc represents a probabilistic dependence. If an arc is drawn from a node Y to a node Z, then Y is a **parent** or **immediate predecessor** of Z, and Z is a **descendant**



(a)

	FH, S	*FH, ~S*	*~FH, S*	*~FH, ~S*
LC	0.8	0.5	0.7	0.1
~LC	0.2	0.5	0.3	0.9

(b)

Figure 9.1 Simple Bayesian belief network. (a) A proposed causal model, represented by a directed acyclic graph. (b) The conditional probability table for the values of the variable *LungCancer* (*LC*) showing each possible combination of the values of its parent nodes, *FamilyHistory* (*FH*) and *Smoker* (*S*). *Source:* Adapted from Russell, Binder, Koller, and Kanazawa [RBKK95].

of Y. *Each variable is conditionally independent of its nondescendants in the graph, given its parents.*

Figure 9.1 is a simple belief network, adapted from Russell, Binder, Koller, and Kanazawa [RBKK95] for six Boolean variables. The arcs in Figure 9.1(a) allow a representation of causal knowledge. For example, having lung cancer is influenced by a person's family history of lung cancer, as well as whether or not the person is a smoker. Note that the variable *PositiveXRay* is independent of whether the patient has a family history of lung cancer or is a smoker, given that we know the patient has lung cancer. In other words, once we know the outcome of the variable *LungCancer*, then the variables *FamilyHistory* and *Smoker* do not provide any additional information regarding *PositiveXRay*. The arcs also show that the variable *LungCancer* is conditionally independent of *Emphysema*, given its parents, *FamilyHistory* and *Smoker*.

A belief network has one **conditional probability table (CPT)** for each variable. The CPT for a variable Y specifies the conditional distribution $P(Y|Parents(Y))$, where $Parents(Y)$ are the parents of Y. Figure 9.1(b) shows a CPT for the variable *LungCancer*. The conditional probability for each known value of *LungCancer* is given for each possible combination of the values of its parents. For instance, from the upper leftmost and bottom rightmost entries, respectively, we see that

$$P(LungCancer = yes\,|\,FamilyHistory = yes,\ Smoker = yes) = 0.8$$

$$P(LungCancer = no\,|\,FamilyHistory = no,\ Smoker = no) = 0.9.$$

Let $\boldsymbol{X} = (x_1, \ldots, x_n)$ be a data tuple described by the variables or attributes $Y_1, \ldots, Y_n$, respectively. Recall that each variable is conditionally independent of its nondescendants in the network graph, given its parents. This allows the network to provide a complete representation of the existing joint probability distribution with the following equation:

$$P(x_1, \ldots, x_n) = \prod_{i=1}^{n} P(x_i|Parents(Y_i)), \tag{9.1}$$

where $P(x_1, \ldots, x_n)$ is the probability of a particular combination of values of $\boldsymbol{X}$, and the values for $P(x_i|Parents(Y_i))$ correspond to the entries in the CPT for Y_i.

A node within the network can be selected as an "output" node, representing a class label attribute. There may be more than one output node. Various algorithms for inference and learning can be applied to the network. Rather than returning a single class label, the classification process can return a probability distribution that gives the probability of each class. Belief networks can be used to answer probability of evidence queries (e.g., what is the probability that an individual will have *LungCancer*, given that they have both *PositiveXRay* and *Dyspnea*) and most probable explanation queries (e.g., which group of the population is most likely to have both *PositiveXRay* and *Dyspnea*).

Belief networks have been used to model a number of well-known problems. One example is genetic linkage analysis (e.g., the mapping of genes onto a chromosome). By casting the gene linkage problem in terms of inference on Bayesian networks, and using state-of-the art algorithms, the scalability of such analysis has advanced considerably. Other applications that have benefited from the use of belief networks include computer vision (e.g., image restoration and stereo vision), document and text analysis, decision-support systems, and sensitivity analysis. The ease with which many applications can be reduced to Bayesian network inference is advantageous in that it curbs the need to invent specialized algorithms for each such application.

9.1.2 Training Bayesian Belief Networks

"*How does a Bayesian belief network learn?*" In the learning or training of a belief network, a number of scenarios are possible. The network **topology** (or "layout" of nodes and arcs) may be constructed by human experts or inferred from the data. The network variables may be *observable* or *hidden* in all or some of the training tuples. The hidden data case is also referred to as *missing values* or *incomplete data.*

Several algorithms exist for learning the network topology from the training data given observable variables. The problem is one of discrete optimization. For solutions, please see the bibliographic notes at the end of this chapter (Section 9.10). Human experts usually have a good grasp of the direct conditional dependencies that hold in the domain under analysis, which helps in network design. Experts must specify conditional probabilities for the nodes that participate in direct dependencies. These probabilities can then be used to compute the remaining probability values.

If the network topology is known and the variables are observable, then training the network is straightforward. It consists of computing the CPT entries, as is similarly done when computing the probabilities involved in naïve Bayesian classification.

When the network topology is given and some of the variables are hidden, there are various methods to choose from for training the belief network. We will describe a promising method of gradient descent. For those without an advanced math background, the description may look rather intimidating with its calculus-packed formulae. However, packaged software exists to solve these equations, and the general idea is easy to follow.

Let D be a training set of data tuples, $\boldsymbol{X}_1, \boldsymbol{X}_2, \ldots, \boldsymbol{X}_{|D|}$. Training the belief network means that we must learn the values of the CPT entries. Let w_{ijk} be a CPT entry for the variable $Y_i = y_{ij}$ having the parents $U_i = u_{ik}$, where $w_{ijk} \equiv P(Y_i = y_{ij} | U_i = u_{ik})$. For example, if w_{ijk} is the upper leftmost CPT entry of Figure 9.1(b), then Y_i is *LungCancer*; y_{ij} is its value, "*yes*"; U_i lists the parent nodes of Y_i, namely, {*FamilyHistory, Smoker*}; and u_{ik} lists the values of the parent nodes, namely, {"*yes*", "*yes*"}. The w_{ijk} are viewed as weights, analogous to the weights in hidden units of neural networks (Section 9.2). The set of weights is collectively referred to as $\boldsymbol{W}$. The weights are initialized to random probability values. A *gradient descent* strategy performs greedy hill-climbing. At each iteration, the weights are updated and will eventually converge to a local optimum solution.

A **gradient descent** strategy is used to search for the w_{ijk} values that best model the data, based on the assumption that each possible setting of w_{ijk} is equally likely. Such a strategy is iterative. It searches for a solution along the negative of the gradient (i.e., steepest descent) of a criterion function. We want to find the set of weights, $\boldsymbol{W}$, that maximize this function. To start with, the weights are initialized to random probability values. The gradient descent method performs greedy hill-climbing in that, at each iteration or step along the way, the algorithm moves toward what appears to be the best solution at the moment, without backtracking. The weights are updated at each iteration. Eventually, they converge to a local optimum solution.

For our problem, we maximize $P_w(D) = \prod_{d=1}^{|D|} P_w(\boldsymbol{X}_d)$. This can be done by following the gradient of $\ln P_w(S)$, which makes the problem simpler. Given the network topology and initialized w_{ijk}, the algorithm proceeds as follows:

1. **Compute the gradients:** For each i, j, k, compute

$$\frac{\partial \ln P_w(D)}{\partial w_{ijk}} = \sum_{d=1}^{|D|} \frac{P(Y_i = y_{ij}, U_i = u_{ik} | \boldsymbol{X}_d)}{w_{ijk}}. \tag{9.2}$$

   The probability on the right side of Eq. (9.2) is to be calculated for each training tuple, $\boldsymbol{X}_d$, in D. For brevity, let's refer to this probability simply as p. When the variables represented by Y_i and U_i are hidden for some $\boldsymbol{X}_d$, then the corresponding probability p can be computed from the observed variables of the tuple using standard algorithms for Bayesian network inference such as those available in the commercial software package HUGIN (*www.hugin.dk*).

2. **Take a small step in the direction of the gradient:** The weights are updated by

$$w_{ijk} \leftarrow w_{ijk} + (l) \frac{\partial \ln P_w(D)}{\partial w_{ijk}}, \tag{9.3}$$

   where l is the **learning rate** representing the step size and $\frac{\partial \ln P_w(D)}{\partial w_{ijk}}$ is computed from Eq. (9.2). The learning rate is set to a small constant and helps with convergence.

3. **Renormalize the weights:** Because the weights w_{ijk} are probability values, they must be between 0.0 and 1.0, and $\sum_j w_{ijk}$ must equal 1 for all i, k. These criteria are achieved by renormalizing the weights after they have been updated by Eq. (9.3).

Algorithms that follow this learning form are called *adaptive probabilistic networks.* Other methods for training belief networks are referenced in the bibliographic notes at the end of this chapter (Section 9.10). Belief networks are computationally intensive. Because belief networks provide explicit representations of causal structure, a human expert can provide prior knowledge to the training process in the form of network topology and/or conditional probability values. This can significantly improve the learning rate.

9.2 Classification by Backpropagation

"*What is backpropagation?*" Backpropagation is a neural network learning algorithm. The neural networks field was originally kindled by psychologists and neurobiologists who sought to develop and test computational analogs of neurons. Roughly speaking, a **neural network** is a set of connected input/output units in which each connection has a weight associated with it. During the learning phase, the network learns by adjusting the weights so as to be able to predict the correct class label of the input tuples. Neural network learning is also referred to as **connectionist learning** due to the connections between units.

Neural networks involve long training times and are therefore more suitable for applications where this is feasible. They require a number of parameters that are typically best determined empirically such as the network topology or "structure." Neural networks have been criticized for their poor interpretability. For example, it is difficult for humans to interpret the symbolic meaning behind the learned weights and of "hidden units" in the network. These features initially made neural networks less desirable for data mining.

Advantages of neural networks, however, include their high tolerance of noisy data as well as their ability to classify patterns on which they have not been trained. They can be used when you may have little knowledge of the relationships between attributes and classes. They are well suited for continuous-valued inputs *and* outputs, unlike most decision tree algorithms. They have been successful on a wide array of real-world data, including handwritten character recognition, pathology and laboratory medicine, and training a computer to pronounce English text. Neural network algorithms are inherently parallel; parallelization techniques can be used to speed up the computation process. In addition, several techniques have been recently developed for rule extraction from trained neural networks. These factors contribute to the usefulness of neural networks for classification and numeric prediction in data mining.

There are many different kinds of neural networks and neural network algorithms. The most popular neural network algorithm is *backpropagation*, which gained repute in the 1980s. In Section 9.2.1 you will learn about multilayer feed-forward networks, the type of neural network on which the backpropagation algorithm performs. Section 9.2.2 discusses defining a network topology. The backpropagation algorithm is described in Section 9.2.3. Rule extraction from trained neural networks is discussed in Section 9.2.4.

9.2.1 A Multilayer Feed-Forward Neural Network

The backpropagation algorithm performs learning on a *multilayer feed-forward* neural network. It iteratively learns a set of weights for prediction of the class label of tuples. A **multilayer feed-forward** neural network consists of an *input layer*, one or more *hidden layers*, and an *output layer*. An example of a multilayer feed-forward network is shown in Figure 9.2.

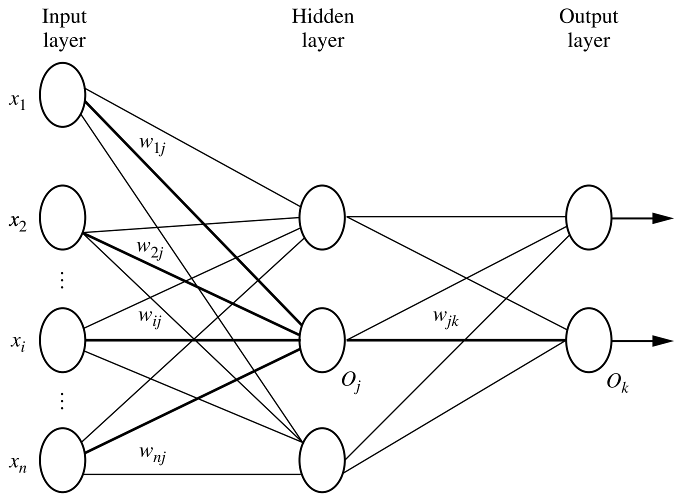


Figure 9.2 Multilayer feed-forward neural network.

Each layer is made up of units. The inputs to the network correspond to the attributes measured for each training tuple. The inputs are fed simultaneously into the units making up the **input layer**. These inputs pass through the input layer and are then weighted and fed simultaneously to a second layer of "neuronlike" units, known as a **hidden layer**. The outputs of the hidden layer units can be input to another hidden layer, and so on. The number of hidden layers is arbitrary, although in practice, usually only one is used. The weighted outputs of the last hidden layer are input to units making up the **output layer**, which emits the network's prediction for given tuples.

The units in the input layer are called **input units**. The units in the hidden layers and output layer are sometimes referred to as **neurodes**, due to their symbolic biological basis, or as **output units**. The multilayer neural network shown in Figure 9.2 has two layers of output units. Therefore, we say that it is a **two-layer** neural network. (The input layer is not counted because it serves only to pass the input values to the next layer.) Similarly, a network containing two hidden layers is called a *three-layer* neural network, and so on. It is a feed-forward network since none of the weights cycles back to an input unit or to a previous layer's output unit. It is **fully connected** in that each unit provides input to each unit in the next forward layer.

Each output unit takes, as input, a weighted sum of the outputs from units in the previous layer (see Figure 9.4 later). It applies a nonlinear (activation) function to the weighted input. Multilayer feed-forward neural networks are able to model the class prediction as a nonlinear combination of the inputs. From a statistical point of view, they perform nonlinear regression. *Multilayer feed-forward networks, given enough hidden units and enough training samples, can closely approximate any function.*

9.2.2 Defining a Network Topology

"*How can I design the neural network's topology?*" Before training can begin, the user must decide on the network topology by specifying the number of units in the input layer, the number of hidden layers (if more than one), the number of units in each hidden layer, and the number of units in the output layer.

Normalizing the input values for each attribute measured in the training tuples will help speed up the learning phase. Typically, input values are normalized so as to fall between 0.0 and 1.0. Discrete-valued attributes may be encoded such that there is one input unit per domain value. For example, if an attribute A has three possible or known values, namely $\{a_0, a_1, a_2\}$, then we may assign three input units to represent A. That is, we may have, say, I_0, I_1, I_2 as input units. Each unit is initialized to 0. If $A = a_0$, then I_0 is set to 1 and the rest are 0. If $A = a_1$, then I_1 is set to 1 and the rest are 0, and so on.

Neural networks can be used for both classification (to predict the class label of a given tuple) and numeric prediction (to predict a continuous-valued output). For classification, one output unit may be used to represent two classes (where the value 1 represents one class, and the value 0 represents the other). If there are more than two classes, then one output unit per class is used. (See Section 9.7.1 for more strategies on multiclass classification.)

There are no clear rules as to the "best" number of hidden layer units. Network design is a trial-and-error process and may affect the accuracy of the resulting trained network. The initial values of the weights may also affect the resulting accuracy. Once a network has been trained and its accuracy is not considered acceptable, it is common to repeat the training process with a different network topology or a different set of initial weights. Cross-validation techniques for accuracy estimation (described in Chapter 8) can be used to help decide when an acceptable network has been found. A number of automated techniques have been proposed that search for a "good" network structure. These typically use a hill-climbing approach that starts with an initial structure that is selectively modified.

9.2.3 Backpropagation

"*How does backpropagation work?*" Backpropagation learns by iteratively processing a data set of training tuples, comparing the network's prediction for each tuple with the actual known *target* value. The target value may be the known class label of the training tuple (for classification problems) or a continuous value (for numeric prediction). For each training tuple, the weights are modified so as to minimize the mean-squared error between the network's prediction and the actual target value. These modifications are made in the "backwards" direction (i.e., from the output layer) through each hidden layer down to the first hidden layer (hence the name *backpropagation*). Although it is not guaranteed, in general the weights will eventually converge, and the learning process stops. The algorithm is summarized in Figure 9.3. The steps involved are expressed in terms of inputs, outputs, and errors, and may seem awkward if this is your first look at

Algorithm: Backpropagation. Neural network learning for classification or numeric prediction, using the backpropagation algorithm.

Input:

- D, a data set consisting of the training tuples and their associated target values;
- l, the learning rate;
- *network*, a multilayer feed-forward network.

Output: A trained neural network.

Method:

```
(1)  Initialize all weights and biases in network;
(2)  while terminating condition is not satisfied {
(3)      for each training tuple $X$ in $D$ {
(4)          // Propagate the inputs forward:
(5)          for each input layer unit $j$ {
(6)              $O_j = I_j$; // output of an input unit is its actual input value
(7)          for each hidden or output layer unit $j$ {
(8)              $I_j = \sum_i w_{ij} O_i + \theta_j$; //compute the net input of unit $j$ with respect to
                     the previous layer, $i$
(9)              $O_j = \frac{1}{1+e^{-I_j}}$; } // compute the output of each unit $j$
(10)         // Backpropagate the errors:
(11)         for each unit $j$ in the output layer
(12)             $Err_j = O_j(1 - O_j)(T_j - O_j)$; // compute the error
(13)         for each unit $j$ in the hidden layers, from the last to the first hidden layer
(14)             $Err_j = O_j(1 - O_j) \sum_k Err_k w_{jk}$; // compute the error with respect to
                     the next higher layer, $k$
(15)         for each weight $w_{ij}$ in network {
(16)             $\Delta w_{ij} = (l) Err_j O_i$; // weight increment
(17)             $w_{ij} = w_{ij} + \Delta w_{ij}$; } // weight update
(18)         for each bias $\theta_j$ in network {
(19)             $\Delta \theta_j = (l) Err_j$; // bias increment
(20)             $\theta_j = \theta_j + \Delta \theta_j$; } // bias update
(21)         } }
```

Figure 9.3 Backpropagation algorithm.

neural network learning. However, once you become familiar with the process, you will see that each step is inherently simple. The steps are described next.

Initialize the weights: The weights in the network are initialized to small random numbers (e.g., ranging from −1.0 to 1.0, or −0.5 to 0.5). Each unit has a *bias* associated with it, as explained later. The biases are similarly initialized to small random numbers.

Each training tuple, $\boldsymbol{X}$, is processed by the following steps.

Propagate the inputs forward: First, the training tuple is fed to the network's input layer. The inputs pass through the input units, unchanged. That is, for an input unit, j,

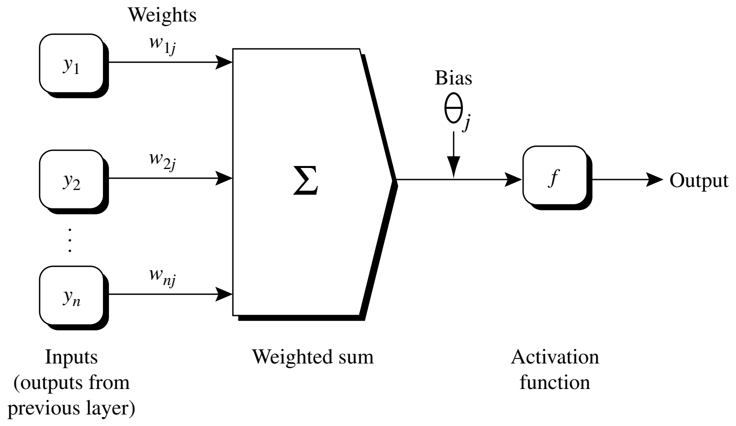


Figure 9.4 Hidden or output layer unit j: The inputs to unit j are outputs from the previous layer. These are multiplied by their corresponding weights to form a weighted sum, which is added to the bias associated with unit j. A nonlinear activation function is applied to the net input. (For ease of explanation, the inputs to unit j are labeled $y_1, y_2, \ldots, y_n$. If unit j were in the first hidden layer, then these inputs would correspond to the input tuple $(x_1, x_2, \ldots, x_n)$.)

its output, O_j, is equal to its input value, I_j. Next, the net input and output of each unit in the hidden and output layers are computed. The net input to a unit in the hidden or output layers is computed as a linear combination of its inputs. To help illustrate this point, a hidden layer or output layer unit is shown in Figure 9.4. Each such unit has a number of inputs to it that are, in fact, the outputs of the units connected to it in the previous layer. Each connection has a weight. To compute the net input to the unit, each input connected to the unit is multiplied by its corresponding weight, and this is summed. Given a unit, j in a hidden or output layer, the net input, I_j, to unit j is

$$I_j = \sum_i w_{ij} O_i + \theta_j, \tag{9.4}$$

where w_{ij} is the weight of the connection from unit i in the previous layer to unit j; O_i is the output of unit i from the previous layer; and θ_j is the **bias** of the unit. The bias acts as a threshold in that it serves to vary the activity of the unit.

Each unit in the hidden and output layers takes its net input and then applies an **activation** function to it, as illustrated in Figure 9.4. The function symbolizes the activation of the neuron represented by the unit. The **logistic**, or **sigmoid**, function is used. Given the net input I_j to unit j, then O_j, the output of unit j, is computed as

$$O_j = \frac{1}{1 + e^{-I_j}}. \tag{9.5}$$

This function is also referred to as a *squashing function*, because it maps a large input domain onto the smaller range of 0 to 1. The logistic function is nonlinear and differentiable, allowing the backpropagation algorithm to model classification problems that are linearly inseparable.

We compute the output values, O_j, for each hidden layer, up to and including the output layer, which gives the network's prediction. In practice, it is a good idea to cache (i.e., save) the intermediate output values at each unit as they are required again later when backpropagating the error. This trick can substantially reduce the amount of computation required.

Backpropagate the error: The error is propagated backward by updating the weights and biases to reflect the error of the network's prediction. For a unit j in the output layer, the error Err_j is computed by

$$Err_j = O_j(1 - O_j)(T_j - O_j), \tag{9.6}$$

where O_j is the actual output of unit j, and T_j is the known target value of the given training tuple. Note that $O_j(1 - O_j)$ is the derivative of the logistic function.

To compute the error of a hidden layer unit j, the weighted sum of the errors of the units connected to unit j in the next layer are considered. The error of a hidden layer unit j is

$$Err_j = O_j(1 - O_j) \sum_k Err_k w_{jk}, \tag{9.7}$$

where w_{jk} is the weight of the connection from unit j to a unit k in the next higher layer, and Err_k is the error of unit k.

The weights and biases are updated to reflect the propagated errors. Weights are updated by the following equations, where Δw_{ij} is the change in weight w_{ij}:

$$\Delta w_{ij} = (l) Err_j O_i. \tag{9.8}$$

$$w_{ij} = w_{ij} + \Delta w_{ij}. \tag{9.9}$$

"*What is* l *in Eq. (9.8)?*" The variable l is the **learning rate**, a constant typically having a value between 0.0 and 1.0. Backpropagation learns using a gradient descent method to search for a set of weights that fits the training data so as to minimize the mean-squared distance between the network's class prediction and the known target value of the tuples.[1] The learning rate helps avoid getting stuck at a local minimum in decision space (i.e., where the weights appear to converge, but are not the optimum solution) and encourages finding the global minimum. If the learning rate is too small, then learning will occur at a very slow pace. If the learning rate is too large, then oscillation between

[1]A method of gradient descent was also used for training Bayesian belief networks, as described in Section 9.1.2.

inadequate solutions may occur. A rule of thumb is to set the learning rate to $1/t$, where t is the number of iterations through the training set so far.

Biases are updated by the following equations, where $\Delta\theta_j$ is the change in bias θ_j:

$$\Delta\theta_j = (l)Err_j. \tag{9.10}$$

$$\theta_j = \theta_j + \Delta\theta_j. \tag{9.11}$$

Note that here we are updating the weights and biases after the presentation of each tuple. This is referred to as **case updating**. Alternatively, the weight and bias increments could be accumulated in variables, so that the weights and biases are updated after all the tuples in the training set have been presented. This latter strategy is called **epoch updating**, where one iteration through the training set is an **epoch**. In theory, the mathematical derivation of backpropagation employs epoch updating, yet in practice, case updating is more common because it tends to yield more accurate results.

Terminating condition: Training stops when

- All Δw_{ij} in the previous epoch are so small as to be below some specified threshold, or
- The percentage of tuples misclassified in the previous epoch is below some threshold, or
- A prespecified number of epochs has expired.

In practice, several hundreds of thousands of epochs may be required before the weights will converge.

"*How efficient is backpropagation?*" The computational efficiency depends on the time spent training the network. Given $|D|$ tuples and w weights, each epoch requires $O(|D| \times w)$ time. However, in the worst-case scenario, the number of epochs can be exponential in n, the number of inputs. In practice, the time required for the networks to converge is highly variable. A number of techniques exist that help speed up the training time. For example, a technique known as *simulated annealing* can be used, which also ensures convergence to a global optimum.

Example 9.1 **Sample calculations for learning by the backpropagation algorithm.** Figure 9.5 shows a multilayer feed-forward neural network. Let the learning rate be 0.9. The initial weight and bias values of the network are given in Table 9.1, along with the first training tuple, $\boldsymbol{X} = (1, 0, 1)$, with a class label of 1.

This example shows the calculations for backpropagation, given the first training tuple, $\boldsymbol{X}$. The tuple is fed into the network, and the net input and output of each unit are computed. These values are shown in Table 9.2. The error of each unit is computed and propagated backward. The error values are shown in Table 9.3. The weight and bias updates are shown in Table 9.4. ■

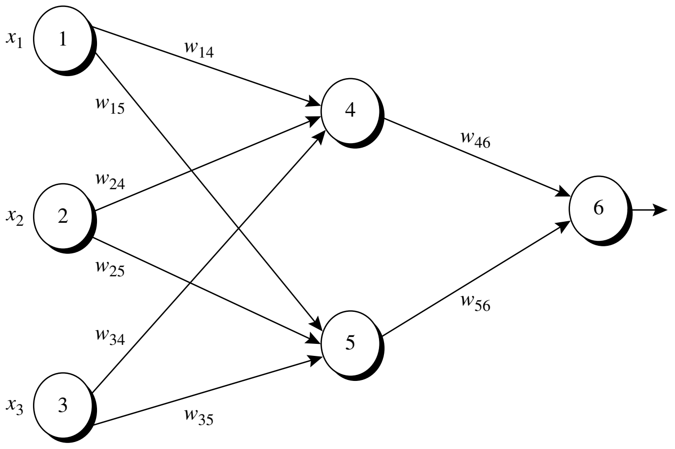


Figure 9.5 Example of a multilayer feed-forward neural network.

Table 9.1 Initial Input, Weight, and Bias Values

x_1	x_2	x_3	w_{14}	w_{15}	w_{24}	w_{25}	w_{34}	w_{35}	w_{46}	w_{56}	θ_4	θ_5	θ_6
1	0	1	0.2	−0.3	0.4	0.1	−0.5	0.2	−0.3	−0.2	−0.4	0.2	0.1

Table 9.2 Net Input and Output Calculations

Unit, j	*Net Input, I_j*	*Output, O_j*
4	$0.2 + 0 - 0.5 - 0.4 = -0.7$	$1/(1 + e^{0.7}) = 0.332$
5	$-0.3 + 0 + 0.2 + 0.2 = 0.1$	$1/(1 + e^{-0.1}) = 0.525$
6	$(-0.3)(0.332) - (0.2)(0.525) + 0.1 = -0.105$	$1/(1 + e^{0.105}) = 0.474$

Table 9.3 Calculation of the Error at Each Node

Unit, j	*Err_j*
6	$(0.474)(1 - 0.474)(1 - 0.474) = 0.1311$
5	$(0.525)(1 - 0.525)(0.1311)(-0.2) = -0.0065$
4	$(0.332)(1 - 0.332)(0.1311)(-0.3) = -0.0087$

Table 9.4 Calculations for Weight and Bias Updating

Weight or Bias	*New Value*
w_{46}	$-0.3 + (0.9)(0.1311)(0.332) = -0.261$
w_{56}	$-0.2 + (0.9)(0.1311)(0.525) = -0.138$
w_{14}	$0.2 + (0.9)(-0.0087)(1) = 0.192$
w_{15}	$-0.3 + (0.9)(-0.0065)(1) = -0.306$
w_{24}	$0.4 + (0.9)(-0.0087)(0) = 0.4$
w_{25}	$0.1 + (0.9)(-0.0065)(0) = 0.1$
w_{34}	$-0.5 + (0.9)(-0.0087)(1) = -0.508$
w_{35}	$0.2 + (0.9)(-0.0065)(1) = 0.194$
θ_6	$0.1 + (0.9)(0.1311) = 0.218$
θ_5	$0.2 + (0.9)(-0.0065) = 0.194$
θ_4	$-0.4 + (0.9)(-0.0087) = -0.408$

"*How can we classify an unknown tuple using a trained network?*" To classify an unknown tuple, ***X***, the tuple is input to the trained network, and the net input and output of each unit are computed. (There is no need for computation and/or backpropagation of the error.) If there is one output node per class, then the output node with the highest value determines the predicted class label for ***X***. If there is only one output node, then output values greater than or equal to 0.5 may be considered as belonging to the positive class, while values less than 0.5 may be considered negative.

Several variations and alternatives to the backpropagation algorithm have been proposed for classification in neural networks. These may involve the dynamic adjustment of the network topology and of the learning rate or other parameters, or the use of different error functions.

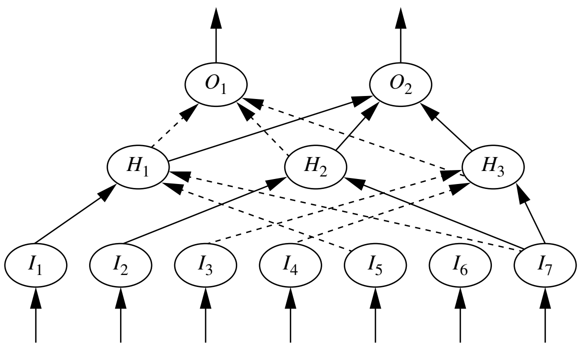
9.2.4 Inside the Black Box: Backpropagation and Interpretability

"*Neural networks are like a black box. How can I 'understand' what the backpropagation network has learned?*" A major disadvantage of neural networks lies in their knowledge representation. Acquired knowledge in the form of a network of units connected by weighted links is difficult for humans to interpret. This factor has motivated research in extracting the knowledge embedded in trained neural networks and in representing that knowledge symbolically. Methods include extracting rules from networks and sensitivity analysis.

Various algorithms for rule extraction have been proposed. The methods typically impose restrictions regarding procedures used in training the given neural network, the network topology, and the discretization of input values.

Fully connected networks are difficult to articulate. Hence, often the first step in extracting rules from neural networks is **network pruning**. This consists of simplifying the network structure by removing weighted links that have the least effect on the trained network. For example, a weighted link may be deleted if such removal does not result in a decrease in the classification accuracy of the network.

Once the trained network has been pruned, some approaches will then perform link, unit, or activation value clustering. In one method, for example, clustering is used to find the set of common activation values for each hidden unit in a given trained two-layer neural network (Figure 9.6). The combinations of these activation values for each hidden unit are analyzed. Rules are derived relating combinations of activation values



Identify sets of common activation values for each hidden node, H_i:

for H_1: (–1,0,1)
for H_2: (0,1)
for H_3: (–1,0.24,1)

Derive rules relating common activation values with output nodes, O_j:

IF (H_2=0 AND H_3=–1) OR
(H_1=–1 AND H_2=1 AND H_3=–1) OR
(H_1=–1 AND H_2=0 AND H_3=0.24)
THEN O_1=1, O_2=0
ELSE O_1=0, O_2=1

Derive rules relating input nodes, I_j, to output nodes, O_j:

IF (I_2=0 AND I_7=0) THEN H_2=0
IF (I_4=1 AND I_6=1) THEN H_3=–1
IF (I_5=0) THEN H_3=–1

Obtain rules relating inputs and output classes:

IF (I_2=0 AND I_7=0 AND I_4=1 AND I_6=1) THEN class=1
IF (I_2=0 AND I_7=0 AND I_5=0) THEN class=1

Figure 9.6 Rules can be extracted from training neural networks. *Source:* Adapted from Lu, Setiono, and Liu [LSL95].

with corresponding output unit values. Similarly, the sets of input values and activation values are studied to derive rules describing the relationship between the input layer and the hidden "layer units"? Finally, the two sets of rules may be combined to form IF-THEN rules. Other algorithms may derive rules of other forms, including M-of-N rules (where M out of a given N conditions in the rule antecedent must be true for the rule consequent to be applied), decision trees with M-of-N tests, fuzzy rules, and finite automata.

Sensitivity analysis is used to assess the impact that a given input variable has on a network output. The input to the variable is varied while the remaining input variables are fixed at some value. Meanwhile, changes in the network output are monitored. The knowledge gained from this analysis form can be represented in rules such as "*IF X decreases* 5% *THEN Y increases* 8%."

9.3 Support Vector Machines

In this section, we study **support vector machines (SVMs)**, a method for the classification of both linear and nonlinear data. In a nutshell, an **SVM** is an algorithm that works as follows. It uses a nonlinear mapping to transform the original training data into a higher dimension. Within this new dimension, it searches for the linear optimal separating hyperplane (i.e., a "decision boundary" separating the tuples of one class from another). With an appropriate nonlinear mapping to a sufficiently high dimension, data from two classes can always be separated by a hyperplane. The SVM finds this hyperplane using *support vectors* ("essential" training tuples) and *margins* (defined by the support vectors). We will delve more into these new concepts later.

"*I've heard that SVMs have attracted a great deal of attention lately. Why?*" The first paper on support vector machines was presented in 1992 by Vladimir Vapnik and colleagues Bernhard Boser and Isabelle Guyon, although the groundwork for SVMs has been around since the 1960s (including early work by Vapnik and Alexei Chervonenkis on statistical learning theory). Although the training time of even the fastest SVMs can be extremely slow, they are highly accurate, owing to their ability to model complex nonlinear decision boundaries. They are much less prone to overfitting than other methods. The support vectors found also provide a compact description of the learned model. SVMs can be used for numeric prediction as well as classification. They have been applied to a number of areas, including handwritten digit recognition, object recognition, and speaker identification, as well as benchmark time-series prediction tests.

9.3.1 The Case When the Data Are Linearly Separable

To explain the mystery of SVMs, let's first look at the simplest case—a two-class problem where the classes are linearly separable. Let the data set D be given as $(\boldsymbol{X}_1, y_1)$, $(\boldsymbol{X}_2, y_2), \ldots, (\boldsymbol{X}_{|D|}, y_{|D|})$, where $\boldsymbol{X}_i$ is the set of training tuples with associated class labels, y_i. Each y_i can take one of two values, either $+1$ or -1 (i.e., $y_i \in \{+1, -1\}$),

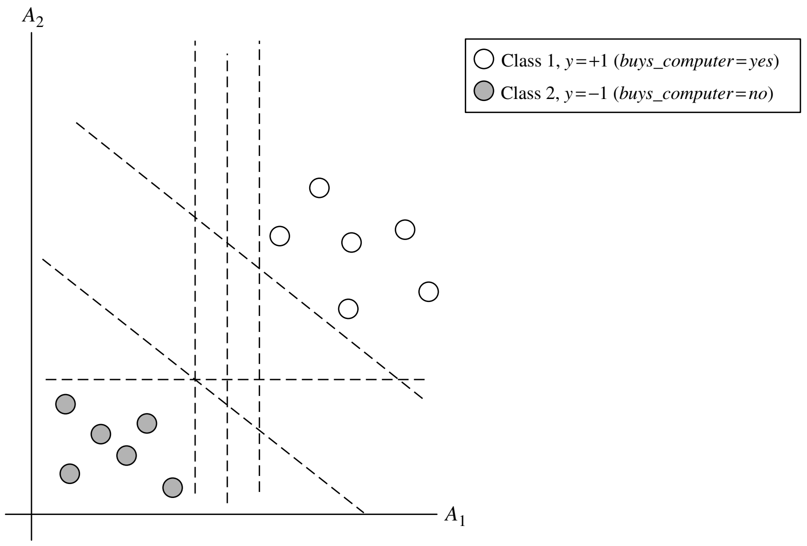
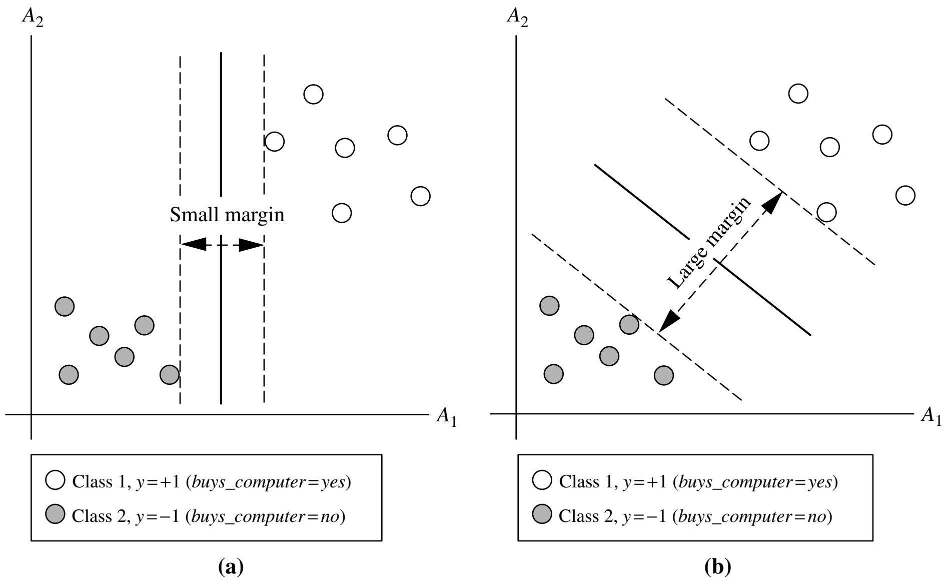


Figure 9.7 The 2-D training data are linearly separable. There are an infinite number of possible separating hyperplanes or "decision boundaries," some of which are shown here as dashed lines. Which one is best?

corresponding to the classes *buys_computer* = *yes* and *buys_computer* = *no*, respectively. To aid in visualization, let's consider an example based on two input attributes, A_1 and A_2, as shown in Figure 9.7. From the graph, we see that the 2-D data are **linearly separable** (or "linear," for short), because a straight line can be drawn to separate all the tuples of class $+1$ from all the tuples of class -1.

There are an infinite number of separating lines that could be drawn. We want to find the "best" one, that is, one that (we hope) will have the minimum classification error on previously unseen tuples. How can we find this best line? Note that if our data were 3-D (i.e., with three attributes), we would want to find the best separating *plane*. Generalizing to n dimensions, we want to find the best *hyperplane*. We will use "hyperplane" to refer to the decision boundary that we are seeking, regardless of the number of input attributes. So, in other words, how can we find the best hyperplane?

An SVM approaches this problem by searching for the **maximum marginal hyperplane**. Consider Figure 9.8, which shows two possible separating hyperplanes and their associated margins. Before we get into the definition of margins, let's take an intuitive look at this figure. Both hyperplanes can correctly classify all the given data tuples. Intuitively, however, we expect the hyperplane with the larger margin to be more accurate at classifying future data tuples than the hyperplane with the smaller margin. This is why (during the learning or training phase) the SVM searches for the hyperplane with the largest margin, that is, the *maximum marginal hyperplane* (MMH). The associated margin gives the largest separation between classes.



A_2
A_1
Small margin
Large margin
Class 1, $y=+1$ (*buys_computer=yes*)
Class 2, $y=-1$ (*buys_computer=no*)
(a)
(b)

Figure 9.8 Here we see just two possible separating hyperplanes and their associated margins. Which one is better? The one with the larger margin (b) should have greater generalization accuracy.

Getting to an informal definition of **margin**, we can say that the shortest distance from a hyperplane to one side of its margin is equal to the shortest distance from the hyperplane to the other side of its margin, where the "sides" of the margin are parallel to the hyperplane. When dealing with the MMH, this distance is, in fact, the shortest distance from the MMH to the closest training tuple of either class.

A separating hyperplane can be written as

$$\boldsymbol{W} \cdot \boldsymbol{X} + b = 0, \tag{9.12}$$

where $\boldsymbol{W}$ is a weight vector, namely, $\boldsymbol{W} = \{w_1, w_2, \ldots, w_n\}$; n is the number of attributes; and b is a scalar, often referred to as a bias. To aid in visualization, let's consider two input attributes, A_1 and A_2, as in Figure 9.8(b). Training tuples are 2-D (e.g., $\boldsymbol{X} = (x_1, x_2)$), where x_1 and x_2 are the values of attributes A_1 and A_2, respectively, for $\boldsymbol{X}$. If we think of b as an additional weight, w_0, we can rewrite Eq. (9.12) as

$$w_0 + w_1x_1 + w_2x_2 = 0. \tag{9.13}$$

Thus, any point that lies above the separating hyperplane satisfies

$$w_0 + w_1x_1 + w_2x_2 > 0. \tag{9.14}$$

Similarly, any point that lies below the separating hyperplane satisfies

$$w_0 + w_1x_1 + w_2x_2 < 0. \tag{9.15}$$

The weights can be adjusted so that the hyperplanes defining the "sides" of the margin can be written as

$$H_1 : w_0 + w_1x_1 + w_2x_2 \geq 1 \quad \text{for } y_i = +1, \tag{9.16}$$

$$H_2 : w_0 + w_1x_1 + w_2x_2 \leq -1 \quad \text{for } y_i = -1. \tag{9.17}$$

That is, any tuple that falls on or above H_1 belongs to class +1, and any tuple that falls on or below H_2 belongs to class −1. Combining the two inequalities of Eqs. (9.16) and (9.17), we get

$$y_i(w_0 + w_1x_1 + w_2x_2) \geq 1, \ \forall i. \tag{9.18}$$

Any training tuples that fall on hyperplanes H_1 or H_2 (i.e., the "sides" defining the margin) satisfy Eq. (9.18) and are called **support vectors**. That is, they are equally close to the (separating) MMH. In Figure 9.9, the support vectors are shown encircled with a thicker border. Essentially, the support vectors are the most difficult tuples to classify and give the most information regarding classification.

From this, we can obtain a formula for the size of the maximal margin. The distance from the separating hyperplane to any point on H_1 is $\frac{1}{||\boldsymbol{W}||}$, where $||\boldsymbol{W}||$ is the Euclidean norm of $\boldsymbol{W}$, that is, $\sqrt{\boldsymbol{W} \cdot \boldsymbol{W}}$.[2] By definition, this is equal to the distance from any point on H_2 to the separating hyperplane. Therefore, the maximal margin is $\frac{2}{||\boldsymbol{W}||}$.

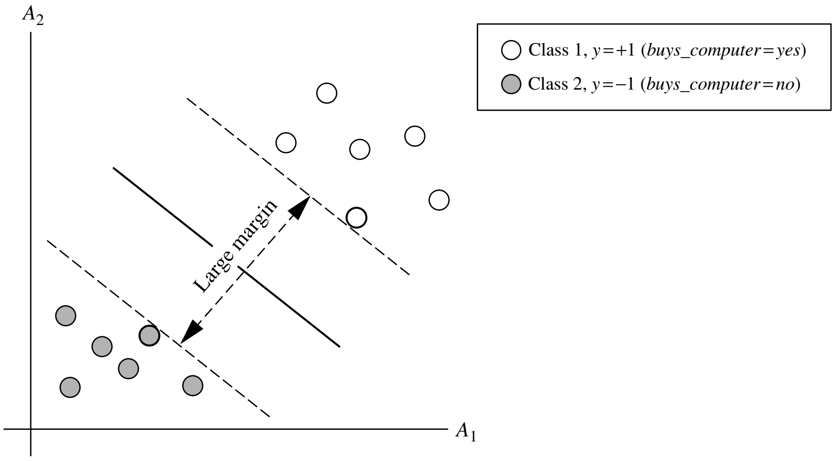

A_2
A_1
Large margin
○ Class 1, y=+1 (*buys_computer*=*yes*)
● Class 2, y=−1 (*buys_computer*=*no*)

Figure 9.9 Support vectors. The SVM finds the maximum separating hyperplane, that is, the one with maximum distance between the nearest training tuples. The support vectors are shown with a thicker border.

[2]If $\boldsymbol{W} = \{w_1, w_2, \ldots, w_n\}$, then $\sqrt{\boldsymbol{W} \cdot \boldsymbol{W}} = \sqrt{w_1^2 + w_2^2 + \cdots + w_n^2}$.

"*So, how does an SVM find the MMH and the support vectors?*" Using some "fancy math tricks," we can rewrite Eq. (9.18) so that it becomes what is known as a constrained (convex) quadratic optimization problem. Such fancy math tricks are beyond the scope of this book. Advanced readers may be interested to note that the tricks involve rewriting Eq. (9.18) using a Lagrangian formulation and then solving for the solution using Karush-Kuhn-Tucker (KKT) conditions. Details can be found in the bibliographic notes at the end of this chapter (Section 9.10).

If the data are small (say, less than 2000 training tuples), any optimization software package for solving constrained convex quadratic problems can then be used to find the support vectors and MMH. For larger data, special and more efficient algorithms for training SVMs can be used instead, the details of which exceed the scope of this book. Once we've found the support vectors and MMH (note that the support vectors define the MMH!), we have a trained support vector machine. The MMH is a linear class boundary, and so the corresponding SVM can be used to classify linearly separable data. We refer to such a trained SVM as a *linear SVM.*

"*Once I've got a trained support vector machine, how do I use it to classify test (i.e., new) tuples?*" Based on the Lagrangian formulation mentioned before, the MMH can be rewritten as the decision boundary

$$d(\boldsymbol{X}^T) = \sum_{i=1}^{l} y_i \alpha_i \boldsymbol{X}_i \boldsymbol{X}^T + b_0, \tag{9.19}$$

where y_i is the class label of support vector $\boldsymbol{X}_i$; $\boldsymbol{X}^T$ is a test tuple; α_i and b_0 are numeric parameters that were determined automatically by the optimization or SVM algorithm noted before; and l is the number of support vectors.

Interested readers may note that the α_i are Lagrangian multipliers. For linearly separable data, the support vectors are a subset of the actual training tuples (although there will be a slight twist regarding this when dealing with nonlinearly separable data, as we shall see in the following).

Given a test tuple, $\boldsymbol{X}^T$, we plug it into Eq. (9.19), and then check to see the sign of the result. This tells us on which side of the hyperplane the test tuple falls. If the sign is positive, then $\boldsymbol{X}^T$ falls on or above the MMH, and so the SVM predicts that $\boldsymbol{X}^T$ belongs to class $+1$ (representing *buys_computer* = *yes*, in our case). If the sign is negative, then $\boldsymbol{X}^T$ falls on or below the MMH and the class prediction is -1 (representing *buys_computer* = *no*).

Notice that the Lagrangian formulation of our problem (Eq. 9.19) contains a dot product between support vector $\boldsymbol{X}_i$ and test tuple $\boldsymbol{X}^T$. This will prove very useful for finding the MMH and support vectors for the case when the given data are nonlinearly separable, as described further in the next section.

Before we move on to the nonlinear case, there are two more important things to note. The complexity of the learned classifier is characterized by the number of support vectors rather than the dimensionality of the data. Hence, SVMs tend to be less prone to overfitting than some other methods. The support vectors are the essential or critical training tuples—they lie closest to the decision boundary (MMH). If all other training tuples were removed and training were repeated, the same separating hyperplane would be found. Furthermore, the number of support vectors found can be used to compute an (upper) bound on the expected error rate of the SVM classifier, which is independent of the data dimensionality. An SVM with a small number of support vectors can have good generalization, even when the dimensionality of the data is high.

9.3.2 The Case When the Data Are Linearly Inseparable

In Section 9.3.1 we learned about linear SVMs for classifying linearly separable data, but what if the data are not linearly separable, as in Figure 9.10? In such cases, no straight line can be found that would separate the classes. The linear SVMs we studied would not be able to find a feasible solution here. Now what?

The good news is that the approach described for linear SVMs can be extended to create *nonlinear SVMs* for the classification of *linearly inseparable data* (also called *nonlinearly separable data*, or *nonlinear data* for short). Such SVMs are capable of finding nonlinear decision boundaries (i.e., nonlinear hypersurfaces) in input space.

"*So,*" you may ask, "*how can we extend the linear approach?*" We obtain a nonlinear SVM by extending the approach for linear SVMs as follows. There are two main steps. In the first step, we transform the original input data into a higher dimensional space using a nonlinear mapping. Several common nonlinear mappings can be used in this step, as we will further describe next. Once the data have been transformed into the new higher space, the second step searches for a linear separating hyperplane in the new space. We again end up with a quadratic optimization problem that can be solved using the linear SVM formulation. The maximal marginal hyperplane found in the new space corresponds to a nonlinear separating hypersurface in the original space.

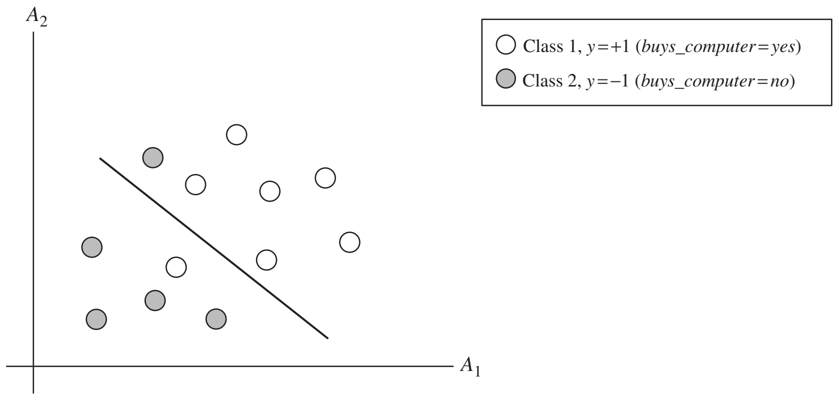


Figure 9.10 A simple 2-D case showing linearly inseparable data. Unlike the linear separable data of Figure 9.7, here it is not possible to draw a straight line to separate the classes. Instead, the decision boundary is nonlinear.

Example 9.2 Nonlinear transformation of original input data into a higher dimensional space. Consider the following example. A 3-D input vector $\boldsymbol{X} = (x_1, x_2, x_3)$ is mapped into a 6-D space, $\boldsymbol{Z}$, using the mappings $\phi_1(\boldsymbol{X}) = x_1$, $\phi_2(\boldsymbol{X}) = x_2$, $\phi_3(\boldsymbol{X}) = x_3$, $\phi_4(\boldsymbol{X}) = (x_1)^2$, $\phi_5(\boldsymbol{X}) = x_1x_2$, and $\phi_6(\boldsymbol{X}) = x_1x_3$. A decision hyperplane in the new space is $d(\boldsymbol{Z}) = \boldsymbol{WZ} + b$, where $\boldsymbol{W}$ and $\boldsymbol{Z}$ are vectors. This is linear. We solve for $\boldsymbol{W}$ and b and then substitute back so that the linear decision hyperplane in the new ($\boldsymbol{Z}$) space corresponds to a nonlinear second-order polynomial in the original 3-D input space:

$$\begin{aligned} d(\boldsymbol{Z}) &= w_1x_1 + w_2x_2 + w_3x_3 + w_4(x_1)^2 + w_5x_1x_2 + w_6x_1x_3 + b \\ &= w_1z_1 + w_2z_2 + w_3z_3 + w_4z_4 + w_5z_5 + w_6z_6 + b. \end{aligned}$$

■

But there are some problems. First, how do we choose the nonlinear mapping to a higher dimensional space? Second, the computation involved will be costly. Refer to Eq. (9.19) for the classification of a test tuple, $\boldsymbol{X^T}$. Given the test tuple, we have to compute its dot product with every one of the support vectors.[3] In training, we have to compute a similar dot product several times in order to find the MMH. This is especially expensive. Hence, the dot product computation required is very heavy and costly. We need another trick!

Luckily, we can use another math trick. It so happens that in solving the quadratic optimization problem of the linear SVM (i.e., when searching for a linear SVM in the new higher dimensional space), the training tuples appear only in the form of dot products, $\phi(\boldsymbol{X}_i) \cdot \phi(\boldsymbol{X}_j)$, where $\phi(\boldsymbol{X})$ is simply the nonlinear mapping function applied to transform the training tuples. Instead of computing the dot product on the transformed data tuples, it turns out that it is mathematically equivalent to instead apply a *kernel function*, $K(\boldsymbol{X}_i, \boldsymbol{X}_j)$, to the original input data. That is,

$$K(\boldsymbol{X}_i, \boldsymbol{X}_j) = \phi(\boldsymbol{X}_i) \cdot \phi(\boldsymbol{X}_j). \tag{9.20}$$

In other words, everywhere that $\phi(\boldsymbol{X}_i) \cdot \phi(\boldsymbol{X}_j)$ appears in the training algorithm, we can replace it with $K(\boldsymbol{X}_i, \boldsymbol{X}_j)$. In this way, all calculations are made in the original input space, which is of potentially much lower dimensionality! We can safely avoid the mapping—it turns out that we don't even have to know what the mapping is! We will talk more later about what kinds of functions can be used as kernel functions for this problem.

After applying this trick, we can then proceed to find a maximal separating hyperplane. The procedure is similar to that described in Section 9.3.1, although it involves placing a user-specified upper bound, C, on the Lagrange multipliers, α_i. This upper bound is best determined experimentally.

"*What are some of the kernel functions that could be used?*" Properties of the kinds of kernel functions that could be used to replace the dot product scenario just described

[3]The dot product of two vectors, $\boldsymbol{X}^T = (x_1^T, x_2^T, \ldots, x_n^T)$ and $\boldsymbol{X}_i = (x_{i1}, x_{i2}, \ldots, x_{in})$ is $x_1^T x_{i1} + x_2^T x_{i2} + \cdots + x_n^T x_{in}$. Note that this involves one multiplication and one addition for each of the n dimensions.

have been studied. Three admissible kernel functions are

Polynomial kernel of degree *h*: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = (\boldsymbol{X}_i \cdot \boldsymbol{X}_j + 1)^h$

Gaussian radial basis function kernel: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = e^{-\|\boldsymbol{X}_i - \boldsymbol{X}_j\|^2/2\sigma^2}$

Sigmoid kernel: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = \tanh(\kappa \boldsymbol{X}_i \cdot \boldsymbol{X}_j - \delta)$

Each of these results in a different nonlinear classifier in (the original) input space. Neural network aficionados will be interested to note that the resulting decision hyperplanes found for nonlinear SVMs are the same type as those found by other well-known neural network classifiers. For instance, an SVM with a Gaussian radial basis function (RBF) gives the same decision hyperplane as a type of neural network known as a radial basis function network. An SVM with a sigmoid kernel is equivalent to a simple two-layer neural network known as a multilayer perceptron (with no hidden layers).

There are no golden rules for determining which admissible kernel will result in the most accurate SVM. In practice, the kernel chosen does not generally make a large difference in resulting accuracy. SVM training always finds a global solution, unlike neural networks, such as backpropagation, where many local minima usually exist (Section 9.2.3).

So far, we have described linear and nonlinear SVMs for binary (i.e., two-class) classification. SVM classifiers can be combined for the multiclass case. See Section 9.7.1 for some strategies, such as training one classifier per class and the use of error-correcting codes.

A major research goal regarding SVMs is to improve the speed in training and testing so that SVMs may become a more feasible option for very large data sets (e.g., millions of support vectors). Other issues include determining the best kernel for a given data set and finding more efficient methods for the multiclass case.

9.4 Classification Using Frequent Patterns

Frequent patterns show interesting relationships between attribute–value pairs that occur frequently in a given data set. For example, we may find that the attribute–value pairs *age* = *youth* and *credit* = *OK* occur in 20% of data tuples describing *AllElectronics* customers who buy a computer. We can think of each attribute–value pair as an *item*, so the search for these frequent patterns is known as *frequent pattern mining* or *frequent itemset mining*. In Chapters 6 and 7, we saw how **association rules** are derived from frequent patterns, where the associations are commonly used to analyze the purchasing patterns of customers in a store. Such analysis is useful in many decision-making processes such as product placement, catalog design, and cross-marketing.

In this section, we examine how frequent patterns can be used for classification. Section 9.4.1 explores **associative classification**, where association rules are generated from frequent patterns and used for classification. The general idea is that we can search for strong associations between frequent patterns (conjunctions of attribute–value pairs) and class labels. Section 9.4.2 explores **discriminative frequent pattern–based classification**, where frequent patterns serve as combined features, which are considered in addition to single features when building a classification model. Because frequent patterns explore highly confident associations among multiple attributes, frequent pattern–based classification may overcome some constraints introduced by decision tree induction, which considers only one attribute at a time. Studies have shown many frequent pattern–based classification methods to have greater accuracy and scalability than some traditional classification methods such as C4.5.

9.4.1 Associative Classification

In this section, you will learn about associative classification. The methods discussed are CBA, CMAR, and CPAR.

Before we begin, however, let's look at association rule mining in general. Association rules are mined in a two-step process consisting of *frequent itemset mining* followed by *rule generation*. The first step searches for patterns of attribute–value pairs that occur repeatedly in a data set, where each attribute–value pair is considered an *item*. The resulting attribute–value pairs form *frequent itemsets* (also referred to as *frequent patterns*). The second step analyzes the frequent itemsets to generate association rules. All association rules must satisfy certain criteria regarding their "accuracy" (or *confidence*) and the proportion of the data set that they actually represent (referred to as *support*). For example, the following is an association rule mined from a data set, D, shown with its confidence and support:

$$\begin{aligned} &age = youth \wedge credit = OK \Rightarrow buys\_computer \\ &\qquad = yes\ [support = 20\%,\ confidence = 93\%], \end{aligned} \tag{9.21}$$

where $\wedge$ represents a logical "AND." We will say more about confidence and support later.

More formally, let D be a data set of tuples. Each tuple in D is described by n attributes, $A_1, A_2, \ldots, A_n$, and a class label attribute, A_{class}. All continuous attributes are discretized and treated as categorical (or nominal) attributes. An **item**, p, is an attribute–value pair of the form (A_i, v), where A_i is an attribute taking a value, v. A data tuple $\mathbf{X} = (x_1, x_2, \ldots, x_n)$ satisfies an item, $p = (A_i, v)$, if and only if $x_i = v$, where x_i is the value of the ith attribute of $\mathbf{X}$. Association rules can have any number of items in the rule antecedent (left side) and any number of items in the rule consequent (right side). However, when mining association rules for use in classification, we are only interested in association rules of the form $p_1 \wedge p_2 \wedge \ldots p_l \Rightarrow A_{class} = C$, where the rule antecedent is a conjunction of items, $p_1, p_2, \ldots, p_l$ $(l \le n)$, associated with a class label, C. For a given rule, R, the percentage of tuples in D satisfying the rule antecedent that also have the class label C is called the **confidence** of R.

From a classification point of view, this is akin to rule accuracy. For example, a confidence of 93% for Rule (9.21) means that 93% of the customers in D who are young and have an OK credit rating belong to the class $buys\_computer = yes$. The percentage of tuples in D satisfying the rule antecedent and having class label C is called the **support** of R. A support of 20% for Rule (9.21) means that 20% of the customers in D are young, have an OK credit rating, and belong to the class *buys_computer* = *yes*.

In general, associative classification consists of the following steps:

1. Mine the data for frequent itemsets, that is, find commonly occurring attribute–value pairs in the data.
2. Analyze the frequent itemsets to generate association rules per class, which satisfy confidence and support criteria.
3. Organize the rules to form a rule-based classifier.

Methods of associative classification differ primarily in the approach used for frequent itemset mining and in how the derived rules are analyzed and used for classification. We now look at some of the various methods for associative classification.

One of the earliest and simplest algorithms for associative classification is **CBA** (Classification Based on Associations). CBA uses an iterative approach to frequent itemset mining, similar to that described for Apriori in Section 6.2.1, where multiple passes are made over the data and the derived frequent itemsets are used to generate and test longer itemsets. In general, the number of passes made is equal to the length of the longest rule found. The complete set of rules satisfying minimum confidence and minimum support thresholds are found and then analyzed for inclusion in the classifier. CBA uses a heuristic method to construct the classifier, where the rules are ordered according to decreasing precedence based on their confidence and support. If a set of rules has the same antecedent, then the rule with the highest confidence is selected to represent the set. When classifying a new tuple, the first rule satisfying the tuple is used to classify it. The classifier also contains a default rule, having lowest precedence, which specifies a default class for any new tuple that is not satisfied by any other rule in the classifier. In this way, the set of rules making up the classifier form a *decision list*. In general, CBA was empirically found to be more accurate than C4.5 on a good number of data sets.

CMAR (Classification based on Multiple Association Rules) differs from CBA in its strategy for frequent itemset mining and its construction of the classifier. It also employs several rule pruning strategies with the help of a tree structure for efficient storage and retrieval of rules. CMAR adopts a variant of the *FP-growth* algorithm to find the complete set of rules satisfying the minimum confidence and minimum support thresholds. FP-growth was described in Section 6.2.4. FP-growth uses a tree structure, called an *FP-tree*, to register all the frequent itemset information contained in the given data set, D. This requires only two scans of D. The frequent itemsets are then mined from the FP-tree. CMAR uses an enhanced FP-tree that maintains the distribution of class labels among tuples satisfying each frequent itemset. In this way, it is able to combine rule generation together with frequent itemset mining in a single step.

CMAR employs another tree structure to store and retrieve rules efficiently and to prune rules based on confidence, correlation, and database coverage. Rule pruning strategies are triggered whenever a rule is inserted into the tree. For example, given two rules, $R1$ and $R2$, if the antecedent of $R1$ is more general than that of $R2$ and $conf(R1) \geq conf(R2)$, then $R2$ is pruned. The rationale is that highly specialized rules with low confidence can be pruned if a more generalized version with higher confidence exists. CMAR also prunes rules for which the rule antecedent and class are not positively correlated, based on an χ^2 test of statistical significance.

"*If more than one rule applies, which one do we use?*" As a classifier, CMAR operates differently than CBA. Suppose that we are given a tuple $\boldsymbol{X}$ to classify and that only one rule satisfies or matches $\boldsymbol{X}$.[4] This case is trivial—we simply assign the rule's class label. Suppose, instead, that more than one rule satisfies $\boldsymbol{X}$. These rules form a set, S. Which rule would we use to determine the class label of $\boldsymbol{X}$? CBA would assign the class label of the most confident rule among the rule set, S. CMAR instead considers multiple rules when making its class prediction. It divides the rules into groups according to class labels. All rules within a group share the same class label and each group has a distinct class label.

CMAR uses a weighted χ^2 measure to find the "strongest" group of rules, based on the statistical correlation of rules within a group. It then assigns $\boldsymbol{X}$ the class label of the strongest group. In this way it considers multiple rules, rather than a single rule with highest confidence, when predicting the class label of a new tuple. In experiments, CMAR had slightly higher average accuracy in comparison with CBA. Its runtime, scalability, and use of memory were found to be more efficient.

"*Is there a way to cut down on the number of rules generated?*" CBA and CMAR adopt methods of frequent itemset mining to generate *candidate* association rules, which include all conjunctions of attribute–value pairs (items) satisfying minimum support. These rules are then examined, and a subset is chosen to represent the classifier. However, such methods generate quite a large number of rules. CPAR (Classification based on Predictive Association Rules) takes a different approach to rule generation, based on a rule generation algorithm for classification known as FOIL (Section 8.4.3). FOIL builds rules to distinguish positive tuples (e.g., $buys\_computer = yes$) from negative tuples (e.g., $buys\_computer = no$). For multiclass problems, FOIL is applied to each class. That is, for a class, C, all tuples of class C are considered positive tuples, while the rest are considered negative tuples. Rules are generated to distinguish C tuples from all others. Each time a rule is generated, the positive samples it satisfies (or *covers*) are removed until all the positive tuples in the data set are covered. In this way, fewer rules are generated. CPAR relaxes this step by allowing the covered tuples to remain under consideration, but reducing their weight. The process is repeated for each class. The resulting rules are merged to form the classifier rule set.

During classification, CPAR employs a somewhat different multiple rule strategy than CMAR. If more than one rule satisfies a new tuple, $\boldsymbol{X}$, the rules are divided into groups according to class, similar to CMAR. However, CPAR uses the best k rules of each group to predict the class label of $\boldsymbol{X}$, based on expected accuracy. By considering the best k rules rather than all of a group's rules, it avoids the influence of lower-ranked

[4]If a rule's antecedent satisfies or matches $\boldsymbol{X}$, then we say that the rule satisfies $\boldsymbol{X}$.

rules. CPAR's accuracy on numerous data sets was shown to be close to that of CMAR. However, since CPAR generates far fewer rules than CMAR, it shows much better efficiency with large sets of training data.

In summary, associative classification offers an alternative classification scheme by building rules based on conjunctions of attribute–value pairs that occur frequently in data.

9.4.2 Discriminative Frequent Pattern–Based Classification

From work on associative classification, we see that frequent patterns reflect strong associations between attribute–value pairs (or items) in data and are useful for classification.

"*But just how discriminative are frequent patterns for classification?*" Frequent patterns represent feature combinations. Let's compare the discriminative power of frequent patterns and single features. Figure 9.11 plots the information gain of frequent patterns and single features (i.e., of pattern length 1) for three UCI data sets.[5] The discrimination power of some frequent patterns is higher than that of single features. Frequent patterns map data to a higher dimensional space. They capture more underlying semantics of the data, and thus can hold greater expressive power than single features.

"*Why not consider frequent patterns as combined features, in addition to single features when building a classification model?*" This notion is the basis of **frequent pattern–based classification**—the learning of a classification model in the feature space of single attributes *as well as* frequent patterns. In this way, we transfer the original feature space to a larger space. This will likely increase the chance of including important features.

Let's get back to our earlier question: How discriminative are frequent patterns? Many of the frequent patterns generated in frequent itemset mining are indiscriminative because they are based solely on support, without considering predictive power. That is, by definition, a pattern must satisfy a user-specified minimum support threshold, *min_sup*, to be considered frequent. For example, if *min_sup*, is, say, 5%, a pattern is frequent if it occurs in 5% of the data tuples. Consider Figure 9.12, which plots information gain versus pattern frequency (support) for three UCI data sets. A theoretical upper bound on information gain, which was derived analytically, is also plotted. The figure shows that the discriminative power (assessed here as information gain) of low-frequency patterns is bounded by a small value. This is due to the patterns' limited coverage of the data set. Similarly, the discriminative power of very high-frequency patterns is also bounded by a small value, which is due to their commonness in the data. The upper bound of information gain is a function of pattern frequency. The information gain upper bound increases monotonically with pattern frequency. These observations can be confirmed analytically. Patterns with medium-large supports (e.g., $support = 300$ in Figure 9.12a) may be discriminative or not. Thus, not every frequent pattern is useful.

[5]The University of California at Irvine (UCI) archives several large data sets at *http://kdd.ics.uci.edu/*. These are commonly used by researchers for the testing and comparison of machine learning and data mining algorithms.

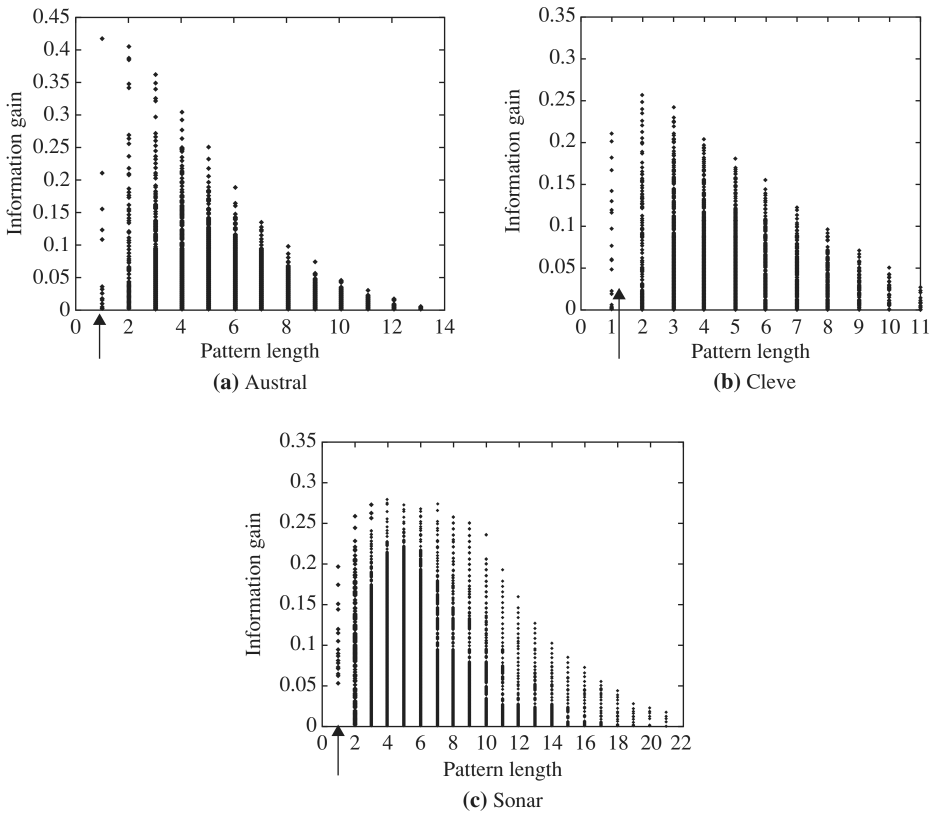


Figure 9.11 Single feature versus frequent pattern: Information gain is plotted for single features (patterns of length 1, indicated by arrows) and frequent patterns (combined features) for three UCI data sets. *Source:* Adapted from Cheng, Yan, Han, and Hsu [CYHH07].

If we were to add all the frequent patterns to the feature space, the resulting feature space would be huge. This slows down the model learning process and may also lead to decreased accuracy due to a form of overfitting in which there are too many features. Many of the patterns may be redundant. Therefore, it's a good idea to apply feature selection to eliminate the less discriminative and redundant frequent patterns as features. The *general framework for discriminative frequent pattern–based classification* is as follows.

1. **Feature generation:** The data, D, are partitioned according to class label. Use frequent itemset mining to discover frequent patterns in each partition, satisfying minimum support. The collection of frequent patterns, $\mathcal{F}$, makes up the feature candidates.

2. **Feature selection:** Apply feature selection to $\mathcal{F}$, resulting in $\mathcal{F}_S$, the set of selected (more discriminating) frequent patterns. Information gain, Fisher score, or other evaluation measures can be used for this step. Relevancy checking can also be

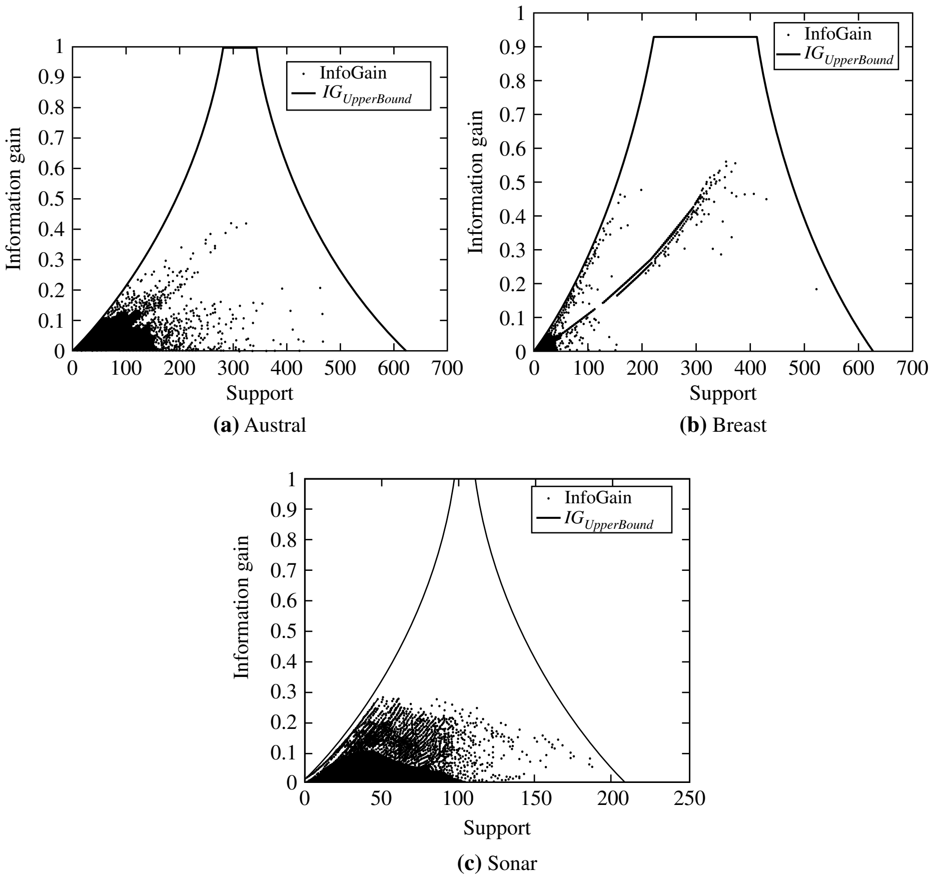


Figure 9.12 Information gain versus pattern frequency (support) for three UCI data sets. A theoretical upper bound on information gain ($IG_{UpperBound}$) is also shown. *Source:* Adapted from Cheng, Yan, Han, and Hsu [CYHH07].

incorporated into this step to weed out redundant patterns. The data set D is transformed to D', where the feature space now includes the single features as well as the selected frequent patterns, $\mathcal{F}_{\mathcal{S}}$.

3. **Learning of classification model:** A classifier is built on the data set D'. Any learning algorithm can be used as the classification model.

The general framework is summarized in Figure 9.13(a), where the discriminative patterns are represented by dark circles. Although the approach is straightforward, we can encounter a computational bottleneck by having to first find *all* the frequent patterns, and then analyze *each one* for selection. The amount of frequent patterns found can be huge due to the explosive number of pattern combinations between items.

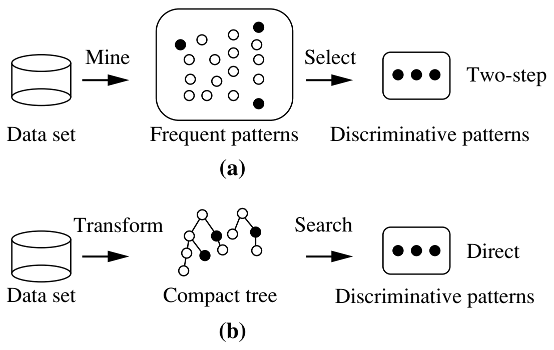


Figure 9.13 A framework for frequent pattern–based classification: (a) a two-step general approach versus (b) the direct approach of DDPMine.

To improve the efficiency of the general framework, consider condensing steps 1 and 2 into just one step. That is, rather than generating the complete set of frequent patterns, it's possible to mine only the highly discriminative ones. This more direct approach is referred to as *direct discriminative pattern mining*. The DDPMine algorithm follows this approach, as illustrated in Figure 9.13(b). It first transforms the training data into a compact tree structure known as a frequent pattern tree, or FP-tree (Section 6.2.4), which holds all of the attribute–value (itemset) association information. It then searches for discriminative patterns on the tree. The approach is direct in that it avoids generating a large number of indiscriminative patterns. It incrementally reduces the problem by eliminating training tuples, thereby progressively shrinking the FP-tree. This further speeds up the mining process.

By choosing to transform the original data to an FP-tree, DDPMine avoids generating redundant patterns because an FP-tree stores only the *closed* frequent patterns. By definition, any subpattern, β, of a closed pattern, α, is redundant with respect to α (Section 6.1.2). DDPMine directly mines the discriminative patterns and integrates feature selection into the mining framework. The theoretical upper bound on information gain is used to facilitate a branch-and-bound search, which prunes the search space significantly. Experimental results show that DDPMine achieves orders of magnitude speedup over the two-step approach without decline in classification accuracy. DDPMine also outperforms state-of-the-art associative classification methods in terms of both accuracy and efficiency.

9.5 Lazy Learners (or Learning from Your Neighbors)

The classification methods discussed so far in this book—decision tree induction, Bayesian classification, rule-based classification, classification by backpropagation, support vector machines, and classification based on association rule mining—are all examples of *eager learners.* **Eager learners**, when given a set of training tuples, will construct a generalization (i.e., classification) model before receiving new (e.g., test) tuples to classify. We can think of the learned model as being ready and eager to classify previously unseen tuples.

Imagine a contrasting lazy approach, in which the learner instead waits until the last minute before doing any model construction to classify a given test tuple. That is, when given a training tuple, a **lazy learner** simply stores it (or does only a little minor processing) and waits until it is given a test tuple. Only when it sees the test tuple does it perform generalization to classify the tuple based on its similarity to the stored training tuples. Unlike eager learning methods, lazy learners do less work when a training tuple is presented and more work when making a classification or numeric prediction. Because lazy learners store the training tuples or "instances," they are also referred to as **instance-based learners**, even though all learning is essentially based on instances.

When making a classification or numeric prediction, lazy learners can be computationally expensive. They require efficient storage techniques and are well suited to implementation on parallel hardware. They offer little explanation or insight into the data's structure. Lazy learners, however, naturally support incremental learning. They are able to model complex decision spaces having hyperpolygonal shapes that may not be as easily describable by other learning algorithms (such as hyperrectangular shapes modeled by decision trees). In this section, we look at two examples of lazy learners: *k-nearest-neighbor classifiers* (Section 9.5.1) and *case-based reasoning classifiers* (Section 9.5.2).

9.5.1 *k*-Nearest-Neighbor Classifiers

The k-nearest-neighbor method was first described in the early 1950s. The method is labor intensive when given large training sets, and did not gain popularity until the 1960s when increased computing power became available. It has since been widely used in the area of pattern recognition.

Nearest-neighbor classifiers are based on learning by analogy, that is, by comparing a given test tuple with training tuples that are similar to it. The training tuples are described by n attributes. Each tuple represents a point in an n-dimensional space. In this way, all the training tuples are stored in an n-dimensional pattern space. When given an unknown tuple, a ***k*-nearest-neighbor classifier** searches the pattern space for the k training tuples that are closest to the unknown tuple. These k training tuples are the k "nearest neighbors" of the unknown tuple.

"Closeness" is defined in terms of a distance metric, such as Euclidean distance. The Euclidean distance between two points or tuples, say, $\boldsymbol{X}_1 = (x_{11}, x_{12}, \ldots, x_{1n})$ and $\boldsymbol{X}_2 = (x_{21}, x_{22}, \ldots, x_{2n})$, is

$$dist(\boldsymbol{X}_1, \boldsymbol{X}_2) = \sqrt{\sum_{i=1}^{n} (x_{1i} - x_{2i})^2}. \tag{9.22}$$

In other words, for each numeric attribute, we take the difference between the corresponding values of that attribute in tuple $\boldsymbol{X}_1$ and in tuple $\boldsymbol{X}_2$, square this difference, and accumulate it. The square root is taken of the total accumulated distance count. Typically, we normalize the values of each attribute before using Eq. (9.22). This helps prevent attributes with initially large ranges (e.g., *income*) from outweighing attributes with initially smaller ranges (e.g., binary attributes). Min-max normalization, for example, can be used to transform a value v of a numeric attribute A to v' in the range [0, 1] by computing

$$v' = \frac{v - min_A}{max_A - min_A}, \tag{9.23}$$

where min_A and max_A are the minimum and maximum values of attribute A. Chapter 3 describes other methods for data normalization as a form of data transformation.

For k-nearest-neighbor classification, the unknown tuple is assigned the most common class among its k-nearest neighbors. When $k = 1$, the unknown tuple is assigned the class of the training tuple that is closest to it in pattern space. Nearest-neighbor classifiers can also be used for numeric prediction, that is, to return a real-valued prediction for a given unknown tuple. In this case, the classifier returns the average value of the real-valued labels associated with the k-nearest neighbors of the unknown tuple.

"*But how can distance be computed for attributes that are not numeric, but nominal (or categorical) such as color?*" The previous discussion assumes that the attributes used to describe the tuples are all numeric. For nominal attributes, a simple method is to compare the corresponding value of the attribute in tuple $\boldsymbol{X}_1$ with that in tuple $\boldsymbol{X}_2$. If the two are identical (e.g., tuples $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$ both have the color blue), then the difference between the two is taken as 0. If the two are different (e.g., tuple $\boldsymbol{X}_1$ is blue but tuple $\boldsymbol{X}_2$ is red), then the difference is considered to be 1. Other methods may incorporate more sophisticated schemes for differential grading (e.g., where a larger difference score is assigned, say, for blue and white than for blue and black).

"*What about missing values?*" In general, if the value of a given attribute A is missing in tuple $\boldsymbol{X}_1$ and/or in tuple $\boldsymbol{X}_2$, we assume the maximum possible difference. Suppose that each of the attributes has been mapped to the range [0, 1]. For nominal attributes, we take the difference value to be 1 if either one or both of the corresponding values of A are missing. If A is numeric and missing from both tuples $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$, then the difference is also taken to be 1. If only one value is missing and the other (which we will call v') is present and normalized, then we can take the difference to be either $|1 - v'|$ or $|0 - v'|$ (i.e., $1 - v'$ or v'), whichever is greater.

"*How can I determine a good value for k, the number of neighbors?*" This can be determined experimentally. Starting with $k = 1$, we use a test set to estimate the error rate of the classifier. This process can be repeated each time by incrementing k to allow for one more neighbor. The k value that gives the minimum error rate may be selected. In general, the larger the number of training tuples, the larger the value of k will be (so that classification and numeric prediction decisions can be based on a larger portion of the stored tuples). As the number of training tuples approaches infinity and $k = 1$, the error rate can be no worse than twice the Bayes error rate (the latter being the theoretical minimum). If k also approaches infinity, the error rate approaches the Bayes error rate.

Nearest-neighbor classifiers use distance-based comparisons that intrinsically assign equal weight to each attribute. They therefore can suffer from poor accuracy when given noisy or irrelevant attributes. The method, however, has been modified to incorporate attribute weighting and the pruning of noisy data tuples. The choice of a distance metric can be critical. The Manhattan (city block) distance (Section 2.4.4), or other distance measurements, may also be used.

Nearest-neighbor classifiers can be extremely slow when classifying test tuples. If D is a training database of $|D|$ tuples and $k = 1$, then $O(|D|)$ comparisons are required to classify a given test tuple. By presorting and arranging the stored tuples into search trees, the number of comparisons can be reduced to $O(log(|D|)$. Parallel implementation can reduce the running time to a constant, that is, $O(1)$, which is independent of $|D|$.

Other techniques to speed up classification time include the use of *partial distance* calculations and *editing* the stored tuples. In the **partial distance** method, we compute the distance based on a subset of the n attributes. If this distance exceeds a threshold, then further computation for the given stored tuple is halted, and the process moves on to the next stored tuple. The **editing** method removes training tuples that prove useless. This method is also referred to as **pruning** or **condensing** because it reduces the total number of tuples stored.

9.5.2 Case-Based Reasoning

Case-based reasoning (CBR) classifiers use a database of problem solutions to solve new problems. Unlike nearest-neighbor classifiers, which store training tuples as points in Euclidean space, CBR stores the tuples or "cases" for problem solving as complex symbolic descriptions. Business applications of CBR include problem resolution for customer service help desks, where cases describe product-related diagnostic problems. CBR has also been applied to areas such as engineering and law, where cases are either technical designs or legal rulings, respectively. Medical education is another area for CBR, where patient case histories and treatments are used to help diagnose and treat new patients.

When given a new case to classify, a case-based reasoner will first check if an identical training case exists. If one is found, then the accompanying solution to that case is returned. If no identical case is found, then the case-based reasoner will search for training cases having components that are similar to those of the new case. Conceptually, these training cases may be considered as neighbors of the new case. If cases are represented as graphs, this involves searching for subgraphs that are similar to subgraphs within the new case. The case-based reasoner tries to combine the solutions of the neighboring training cases to propose a solution for the new case. If incompatibilities arise with the individual solutions, then backtracking to search for other solutions may be necessary. The case-based reasoner may employ background knowledge and problem-solving strategies to propose a feasible combined solution.

Challenges in case-based reasoning include finding a good similarity metric (e.g., for matching subgraphs) and suitable methods for combining solutions. Other challenges include the selection of salient features for indexing training cases and the development of efficient indexing techniques. A trade-off between accuracy and efficiency evolves as the number of stored cases becomes very large. As this number increases, the case-based reasoner becomes more intelligent. After a certain point, however, the system's efficiency will suffer as the time required to search for and process relevant cases increases. As with nearest-neighbor classifiers, one solution is to edit the training database. Cases that are redundant or that have not proved useful may be discarded for the sake of improved performance. These decisions, however, are not clear-cut and their automation remains an active area of research.

9.6 Other Classification Methods

In this section, we give a brief description of several other classification methods, including genetic algorithms (Section 9.6.1), rough set approach (Section 9.6.2), and fuzzy set approaches (Section 9.6.3). In general, these methods are less commonly used for classification in commercial data mining systems than the methods described earlier in this book. However, these methods show their strength in certain applications, and hence it is worthwhile to include them here.

9.6.1 Genetic Algorithms

Genetic algorithms attempt to incorporate ideas of natural evolution. In general, genetic learning starts as follows. An initial **population** is created consisting of randomly generated rules. Each rule can be represented by a string of bits. As a simple example, suppose that samples in a given training set are described by two Boolean attributes, A_1 and A_2, and that there are two classes, C_1 and C_2. The rule "*IF* A_1 *AND NOT* A_2 *THEN* C_2" can be encoded as the bit string "100," where the two leftmost bits represent attributes A_1 and A_2, respectively, and the rightmost bit represents the class. Similarly, the rule "*IF NOT* A_1 *AND NOT* A_2 *THEN* C_1" can be encoded as "001." If an attribute has k values, where $k > 2$, then k bits may be used to encode the attribute's values. Classes can be encoded in a similar fashion.

Based on the notion of survival of the fittest, a new population is formed to consist of the *fittest* rules in the current population, as well as *offspring* of these rules. Typically, the **fitness** of a rule is assessed by its classification accuracy on a set of training samples.

Offspring are created by applying genetic operators such as crossover and mutation. In **crossover**, substrings from pairs of rules are swapped to form new pairs of rules. In **mutation**, randomly selected bits in a rule's string are inverted.

The process of generating new populations based on prior populations of rules continues until a population, P, evolves where each rule in P satisfies a prespecified fitness threshold.

Genetic algorithms are easily parallelizable and have been used for classification as well as other optimization problems. In data mining, they may be used to evaluate the fitness of other algorithms.

9.6.2 Rough Set Approach

Rough set theory can be used for classification to discover structural relationships within imprecise or noisy data. It applies to discrete-valued attributes. Continuous-valued attributes must therefore be discretized before its use.

Rough set theory is based on the establishment of **equivalence classes** within the given training data. All the data tuples forming an equivalence class are indiscernible, that is, the samples are identical with respect to the attributes describing the data. Given real-world data, it is common that some classes cannot be distinguished in terms of the available attributes. Rough sets can be used to approximately or "roughly" define such classes. A rough set definition for a given class, *C*, is approximated by two sets—a **lower approximation** of *C* and an **upper approximation** of *C*. The lower approximation of *C* consists of all the data tuples that, based on the knowledge of the attributes, are certain to belong to *C* without ambiguity. The upper approximation of *C* consists of all the tuples that, based on the knowledge of the attributes, cannot be described as not belonging to *C*. The lower and upper approximations for a class *C* are shown in Figure 9.14, where each rectangular region represents an equivalence class. Decision rules can be generated for each class. Typically, a decision table is used to represent the rules.

Rough sets can also be used for attribute subset selection (or feature reduction, where attributes that do not contribute to the classification of the given training data can be identified and removed) and relevance analysis (where the contribution or significance of each attribute is assessed with respect to the classification task). The problem of finding the minimal subsets (**reducts**) of attributes that can describe all the concepts in the given data set is NP-hard. However, algorithms to reduce the computation intensity have been proposed. In one method, for example, a **discernibility matrix** is used that stores the differences between attribute values for each pair of data tuples. Rather than

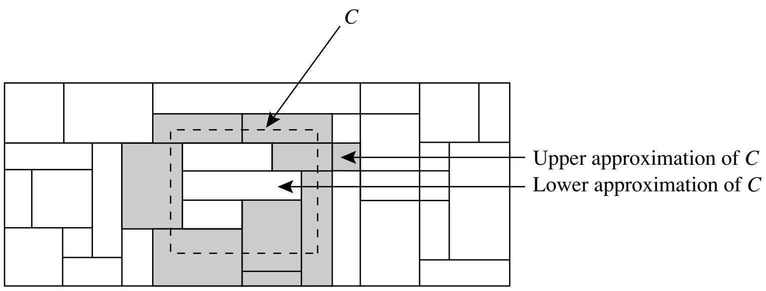


Figure 9.14 A rough set approximation of class *C*'s set of tuples using lower and upper approximation sets of *C*. The rectangular regions represent equivalence classes.

searching on the entire training set, the matrix is instead searched to detect redundant attributes.

9.6.3 Fuzzy Set Approaches

Rule-based systems for classification have the disadvantage that they involve sharp cutoffs for continuous attributes. For example, consider the following rule for customer credit application approval. The rule essentially says that applications for customers who have had a job for two or more years and who have a high income (i.e., of at least \$50,000) are approved:

$$IF\ (years\_employed \geq 2)\ AND\ (income \geq 50{,}000)\ THEN\ credit = approved. \quad (9.24)$$

By Rule (9.24), a customer who has had a job for at least two years will receive credit if her income is, say, \$50,000, but not if it is \$49,000. Such harsh thresholding may seem unfair.

Instead, we can discretize *income* into categories (e.g., {*low_income, medium_income, high_income*}) and then apply **fuzzy logic** to allow "fuzzy" thresholds or boundaries to be defined for each category (Figure 9.15). Rather than having a precise cutoff between categories, fuzzy logic uses truth values between 0.0 and 1.0 to represent the degree of membership that a certain value has in a given category. Each category then represents a **fuzzy set**. Hence, with fuzzy logic, we can capture the notion that an income of \$49,000 is, more or less, high, although not as high as an income of \$50,000. Fuzzy logic systems typically provide graphical tools to assist users in converting attribute values to fuzzy truth values.

Fuzzy set theory is also known as **possibility theory**. It was proposed by Lotfi Zadeh in 1965 as an alternative to traditional two-value logic and probability theory. It lets us work at a high abstraction level and offers a means for dealing with imprecise data

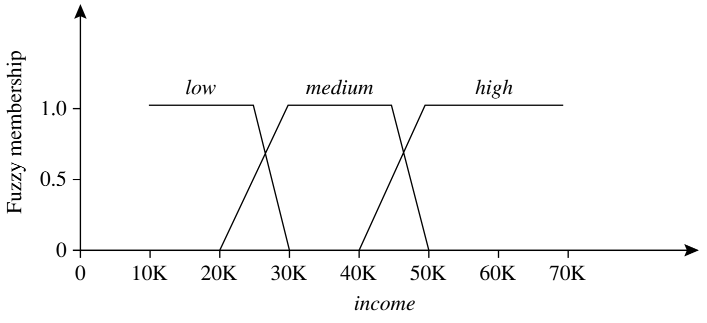


Figure 9.15 Fuzzy truth values for *income*, representing the degree of membership of *income* values with respect to the categories {*low, medium, high*}. Each category represents a fuzzy set. Note that a given income value, x, can have membership in more than one fuzzy set. The membership values of x in each fuzzy set do not have to total to 1.

measurement. Most important, fuzzy set theory allows us to deal with vague or inexact facts. For example, being a member of a set of high incomes is inexact (e.g., if \$50,000 is high, then what about \$49,000? or \$48,000?) Unlike the notion of traditional "crisp" sets where an element belongs to either a set *S* or its complement, in fuzzy set theory, elements can belong to more than one fuzzy set. For example, the income value \$49,000 belongs to both the *medium* and *high* fuzzy sets, but to differing degrees. Using fuzzy set notation and following Figure 9.15, this can be shown as

$$m_{medium\_income}(\$49{,}000) = 0.15 \textit{ and } m_{high\_income}(\$49{,}000) = 0.96,$$

where *m* denotes the membership function, that is operating on the fuzzy sets of *medium_income* and *high_income*, respectively. In fuzzy set theory, membership values for a given element, *x* (e.g., for \$49,000), do not have to sum to 1. This is unlike traditional probability theory, which is constrained by a summation axiom.

Fuzzy set theory is useful for data mining systems performing rule-based classification. It provides operations for combining fuzzy measurements. Suppose that in addition to the fuzzy sets for *income*, we defined the fuzzy sets *junior_employee* and *senior_employee* for the attribute *years_employed*. Suppose also that we have a rule that, say, tests *high_income* and *senior_employee* in the rule antecedent (IF part) for a given employee, *x*. If these two fuzzy measures are ANDed together, the minimum of their measure is taken as the measure of the rule. In other words,

$$m_{(high\_income\ AND\ senior\_employee)}(x) = min(m_{high\_income}(x), m_{senior\_employee}(x)).$$

This is akin to saying that a chain is as strong as its weakest link. If the two measures are ORed, the maximum of their measure is taken as the measure of the rule. In other words,

$$m_{(high\_income\ OR\ senior\_employee)}(x) = max(m_{high\_income}(x), m_{senior\_employee}(x)).$$

Intuitively, this is like saying that a rope is as strong as its strongest strand.

Given a tuple to classify, more than one fuzzy rule may apply. Each applicable rule contributes a vote for membership in the categories. Typically, the truth values for each predicted category are summed, and these sums are combined. Several procedures exist for translating the resulting fuzzy output into a *defuzzified* or crisp value that is returned by the system.

Fuzzy logic systems have been used in numerous areas for classification, including market research, finance, health care, and environmental engineering.

9.7 Additional Topics Regarding Classification

Most of the classification algorithms we have studied handle multiple classes, but some, such as support vector machines, assume only two classes exist in the data. What adaptations can be made to allow for when there are more than two classes? This question is addressed in Section 9.7.1 on *multiclass classification*.

What can we do if we want to build a classifier for data where only some of the data are class-labeled, but most are not? Document classification, speech recognition, and information extraction are just a few examples of applications in which unlabeled data are abundant. Consider *document classification*, for example. Suppose we want to build a model to automatically classify text documents like articles or web pages. In particular, we want the model to distinguish between hockey and football documents. We have a vast amount of documents available, yet the documents are not class-labeled. Recall that supervised learning requires a training set, that is, a set of classlabeled data. To have a human examine and assign a class label to individual documents (to form a training set) is time consuming and expensive.

Speech recognition requires the accurate labeling of speech utterances by trained linguists. It was reported that 1 minute of speech takes 10 minutes to label, and annotating phonemes (basic units of sound) can take 400 times as long. *Information extraction systems* are trained using labeled documents with detailed annotations. These are obtained by having human experts highlight items or relations of interest in text such as the names of companies or individuals. High-level expertise may be required for certain knowledge domains such as gene and disease mentions in biomedical information extraction. Clearly, the manual assignment of class labels to prepare a training set can be extremely costly, time consuming, and tedious.

We study three approaches to classification that are suitable for situations where there is an abundance of unlabeled data. Section 9.7.2 introduces semisupervised classification, which builds a classifier using both labeled and unlabeled data. Section 9.7.3 presents *active learning*, where the learning algorithm carefully selects a few of the unlabeled data tuples and asks a human to label only those tuples. Section 9.7.4 presents *transfer learning*, which aims to extract the knowledge from one or more source tasks (e.g., classifying camera reviews) and apply the knowledge to a target task (e.g., TV reviews). Each of these strategies can reduce the need to annotate large amounts of data, resulting in cost and time savings.

9.7.1 Multiclass Classification

Some classification algorithms, such as support vector machines, are designed for binary classification. How can we extend these algorithms to allow for **multiclass classification** (i.e., classification involving more than two classes)?

A simple approach is **one-versus-all** (OVA). Given m classes, we train m binary classifiers, one for each class. Classifier j is trained using tuples of class j as the positive class, and the remaining tuples as the negative class. It learns to return a positive value for class j and a negative value for the rest. To classify an unknown tuple, $\boldsymbol{X}$, the set of classifiers vote as an ensemble. For example, if classifier j predicts the positive class for $\boldsymbol{X}$, then class j gets one vote. If it predicts the negative class for $\boldsymbol{X}$, then each of the classes except j gets one vote. The class with the most votes is assigned to $\boldsymbol{X}$.

All-versus-all (AVA) is an alternative approach that learns a classifier for each pair of classes. Given m classes, we construct $\frac{m(m-1)}{2}$ binary classifiers. A classifier is trained using tuples of the two classes it should discriminate. To classify an unknown tuple, each classifier votes. The tuple is assigned the class with the maximum number of votes. All-versus-all tends to be superior to one-versus-all.

A problem with the previous schemes is that binary classifiers are sensitive to errors. If any classifier makes an error, it can affect the vote count.

Error-correcting codes can be used to improve the accuracy of multiclass classification, not just in the previous situations, but for classification in general. Error-correcting codes were originally designed to correct errors during data transmission for communication tasks. For such tasks, the codes are used to add redundancy to the data being transmitted so that, even if some errors occur due to noise in the channel, the data can be correctly received at the other end. For multiclass classification, even if some of the individual binary classifiers make a prediction error for a given unknown tuple, we may still be able to correctly label the tuple.

An error-correcting code is assigned to each class, where each code is a bit vector. Figure 9.16 show an example of 7-bit codewords assigned to classes C_1, C_2, C_3, and C_4. We train one classifier for each bit position. Therefore, in our example we train seven classifiers. If a classifier makes an error, there is a better chance that we may still be able to predict the right class for a given unknown tuple because of the redundancy gained by having additional bits. The technique uses a distance measurement called the Hamming distance to guess the "closest" class in case of errors, and is illustrated in Example 9.3.

Example 9.3 **Multiclass classification with error-correcting codes.** Consider the 7-bit codewords associated with classes C_1 to C_4 in Figure 9.16. Suppose that, given an unknown tuple to label, the seven trained binary classifiers collectively output the codeword 0001010, which does not match a codeword for any of the four classes. A classification error has obviously occurred, but can we figure out what the classification most likely should be? We can try by using the **Hamming distance**, which is the number of different bits between two codewords. The Hamming distance between the output codeword and the codeword for C_1 is 5 because five bits—namely, the first, second, third, fifth, and seventh—differ. Similarly, the Hamming distance between the output code and the codewords for C_2 through C_4 are 3, 3, and 1, respectively. Note that the output codeword is closest to the codeword for C_4. That is, the smallest Hamming distance between the output and a class codeword is for class C_4. Therefore, we assign C_4 as the class label of the given tuple. ■

Class	*Error-correcting codeword*
C_1	1 1 1 1 1 1 1
C_2	0 0 0 0 1 1 1
C_3	0 0 1 1 0 0 1
C_4	0 1 0 1 0 1 0

Figure 9.16 Error-correcting codes for a multiclass classification problem involving four classes.

Error-correcting codes can correct up to $\frac{h-1}{h}$ 1-bit errors, where h is the minimum Hamming distance between any two codewords. If we use one bit per class, such as for 4-bit codewords for classes C_1 through C_4, then this is equivalent to the one-versus-all approach, and the codes are not sufficient to self-correct. (Try it as an exercise.) When selecting error-correcting codes for multiclass classification, there must be good row-wise and column-wise separation between the codewords. The greater the distance, the more likely that errors will be corrected.

9.7.2 Semi-Supervised Classification

Semi-supervised classification uses labeled data and unlabeled data to build a classifier. Let $X_l = \{(x_1, y_1), \ldots, x_l, y_l)\}$ be the set of labeled data and $X_u = \{x_{l+1}, \ldots, x_n\}$ be the set of unlabeled data. Here we describe a few examples of this approach for learning.

Self-training is the simplest form of semi-supervised classification. It first builds a classifier using the labeled data. The classifier then tries to label the unlabeled data. The tuple with the most confident label prediction is added to the set of labeled data, and the process repeats (Figure 9.17). Although the method is easy to understand, a disadvantage is that it may reinforce errors.

Cotraining is another form of semi-supervised classification, where two or more classifiers teach each other. Each learner uses a different and ideally independent set of features for each tuple. Consider web page data, for example, where attributes relating to the images on the page may be used as one set of features, while attributes relating to the corresponding text constitute another set of features for the same data. Each set

Self-training

1. Select a learning method such as, say, Bayesian classification. Build the classifier using the labeled data, X_l.
2. Use the classifier to label the unlabeled data, X_u.
3. Select the tuple $x \in X_u$ having the highest confidence (most confident prediction). Add it and its predicted label to X_l.
4. Repeat (i.e., retrain the classifier using the augmented set of labeled data).

Cotraining

1. Define two separate nonoverlapping feature sets for the labeled data, X_l.
2. Train two classifiers, f_1 and f_2, on the labeled data, where f_1 is trained using one of the feature sets and f_2 is trained using the other.
3. Classify X_u with f_1 and f_2 separately.
4. Add the most confident $(x, f_1(x))$ to the set of labeled data used by f_2, where $x \in X_u$. Similarly, add the most confident $(x, f_2(x))$ to the set of labeled data used by f_1.
5. Repeat.

Figure 9.17 Self-training and cotraining methods of semi-supervised classification.

of features should be sufficient to train a good classifier. Suppose we split the feature set into two sets and train two classifiers, f_1 and f_2, where each classifier is trained on a different set. Then, f_1 and f_2 are used to predict the class labels for the unlabeled data, X_u. Each classifier then teaches the other in that the tuple having the most confident prediction from f_1 is added to the set of labeled data for f_2 (along with its label).

Similarly, the tuple having the most confident prediction from f_2 is added to the set of labeled data for f_1. The method is summarized in Figure 9.17. Cotraining is less sensitive to errors than self-training. A difficulty is that the assumptions for its usage may not hold true, that is, it may not be possible to split the features into mutually exclusive and class-conditionally independent sets.

Alternate approaches to semi-supervised learning exist. For example, we can model the joint probability distribution of the features and the labels. For the unlabeled data, the labels can then be treated as missing data. The EM algorithm (Chapter 11) can be used to maximize the likelihood of the model. Methods using support vector machines have also been proposed.

9.7.3 Active Learning

Active learning is an iterative type of supervised learning that is suitable for situations where data are abundant, yet the class labels are scarce or expensive to obtain. The learning algorithm is active in that it can purposefully query a user (e.g., a human oracle) for labels. The number of tuples used to learn a concept this way is often much smaller than the number required in typical supervised learning.

"*How does active learning work to overcome the labeling bottleneck?*" To keep costs down, the active learner aims to achieve high accuracy using as few labeled instances as possible. Let D be all of data under consideration. Various strategies exist for active learning on D. Figure 9.18 illustrates a *pool-based approach* to active learning. Suppose that a small subset of D is class-labeled. This set is denoted L. U is the set of unlabeled data in D. It is also referred to as a pool of unlabeled data. An active learner begins with L as the initial training set. It then uses a *querying function* to carefully select one or more data samples from U and requests labels for them from an oracle (e.g., a human annotator). The newly labeled samples are added to L, which the learner then uses in a standard supervised way. The process repeats. The active learning goal is to achieve high accuracy using as few labeled tuples as possible. Active learning algorithms are typically evaluated with the use of learning curves, which plot accuracy as a function of the number of instances queried.

Most of the active learning research focuses on how to *choose* the data tuples to be queried. Several frameworks have been proposed. *Uncertainty sampling* is the most common, where the active learner chooses to query the tuples which it is the least certain how to label. Other strategies work to reduce the *version space*, that is, the subset of all hypotheses that are consistent with the observed training tuples. Alternatively, we may follow a decision-theoretic approach that estimates expected error reduction. This selects tuples that would result in the greatest reduction in the total number of

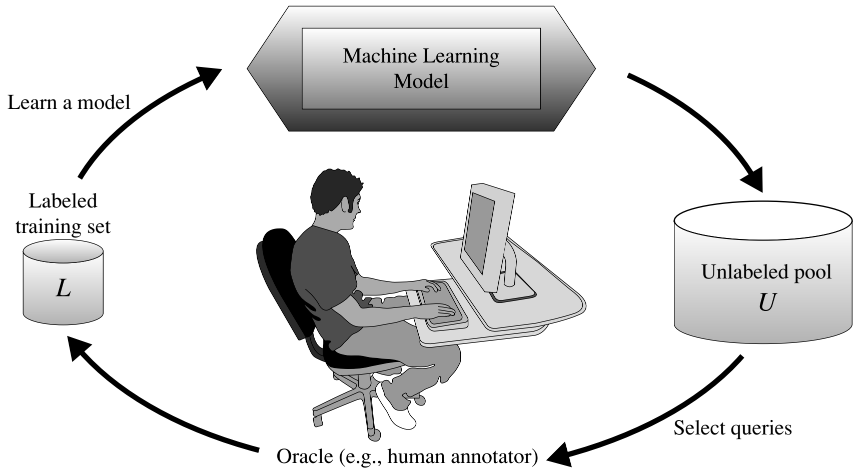


Figure 9.18 The pool-based active learning cycle. *Source:* From Settles [Set10], Burr Settles Computer Sciences Technical Report 1648, University of Wisconsin–Madison; used with permission.

incorrect predictions such as by reducing the expected entropy over U. This latter approach tends to be more computationally expensive.

9.7.4 Transfer Learning

Suppose that *AllElectronics* has collected a number of customer reviews on a product such as a brand of camera. The classification task is to automatically label the reviews as either positive or negative. This task is known as **sentiment classification**. We could examine each review and annotate it by adding a *positive* or *negative* class label. The labeled reviews can then be used to train and test a classifier to label future reviews of the product as either positive or negative. The manual effort involved in annotating the review data can be expensive and time consuming.

Suppose that *AllElectronics* has customer reviews for other products as well such as TVs. The distribution of review data for different types of products can vary greatly. We cannot assume that the TV-review data will have the same distribution as the camera-review data; thus we must build a separate classification model for the TV-review data. Examining and labeling the TV-review data to form a training set will require a lot of effort. In fact, we would need to label a large amount of the data to train the review-classification models for each product. It would be nice if we could adapt an existing classification model (e.g., the one we built for cameras) to help learn a classification model for TVs. Such *knowledge transfer* would reduce the need to annotate a large amount of data, resulting in cost and time savings. This is the essence behind *transfer learning.*

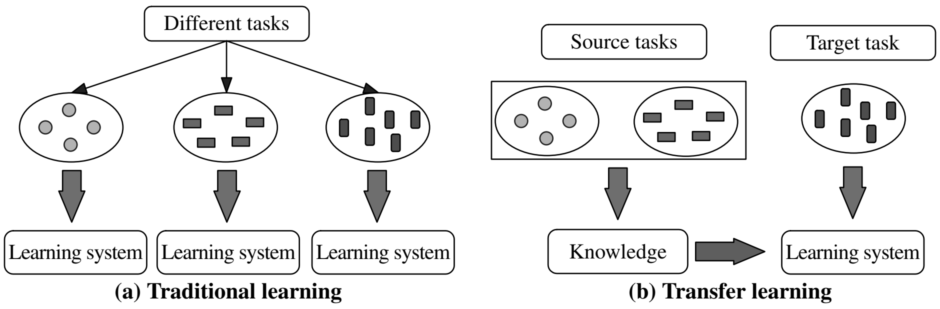


Figure 9.19 Transfer learning versus traditional learning. (a) Traditional learning methods build a new classifier from scratch for each classification task. (b) Transfer learning applies knowledge from a source classifier to simplify the construction of a classifier for a new, target task. *Source:* From Pan and Yang [PY10]; used with permission.

Transfer learning aims to extract the knowledge from one or more *source tasks* and apply the knowledge to a *target task*. In our example, the source task is the classification of camera reviews, and the target task is the classification of TV reviews. Figure 9.19 illustrates a comparison between traditional learning methods and transfer learning. Traditional learning methods build a new classifier for each new classification task, based on available class-labeled training and test data. Transfer learning algorithms apply knowledge about source tasks when building a classifier for a new (target) task. Construction of the resulting classifier requires fewer training data and less training time. Traditional learning algorithms assume that the training data and test data are drawn from the same distribution and the same feature space. Thus, if the distribution changes, such methods need to rebuild the models from scratch.

Transfer learning allows the distributions, tasks, and even the data domains used in training and testing to be different. Transfer learning is analogous to the way humans may apply their knowledge of a task to facilitate the learning of another task. For example, if we know how to play the recorder, we may apply our knowledge of note reading and music to simplify the task of learning to play the piano. Similarly, knowing Spanish may make it easier to learn Italian.

Transfer learning is useful for common applications where the data become outdated or the distribution changes. Here we give two more examples. Consider *web-document classification*, where we may have trained a classifier to label, say, articles from various newsgroups according to predefined categories. The web data that were used to train the classifier can easily become outdated because the topics on the Web change frequently. Another application area for transfer learning is *email spam filtering*. We could train a classifier to label email as either "*spam*" or "*not spam*," using email from a group of users. If new users come along, the distribution of their email can be different from the original group, hence the need to adapt the learned model to incorporate the new data.

There are various approaches to transfer learning, the most common of which is the *instance-based transfer learning* approach. This approach reweights some of the data from the source task and uses it to learn the target task. The **TrAdaBoost** (Transfer AdaBoost) algorithm exemplifies this approach. Consider our previous example of web-document classification, where the distribution of the old data on which the classifier was trained (the source data) is different from the newer data (the target data). TrAdaBoost assumes that the source and target domain data are each described by the same set of attributes (i.e., they have the same "feature space") and the same set of class labels, but that the distribution of the data in the two domains is very different. It extends the AdaBoost ensemble method described in Section 8.6.3. TrAdaBoost requires the labeling of only a small amount of the target data. Rather than throwing out all the old source data, TrAdaBoost assumes that a large amount of it can be useful in training the new classification model. The idea is to filter out the influence of any old data that are very different from the new data by automatically adjusting weights assigned to the training tuples.

Recall that in boosting, an ensemble is created by learning a series of classifiers. To begin, each tuple is assigned a weight. After a classifier M_i is learned, the weights are updated to allow the subsequent classifier, M_{i+1}, to "pay more attention" to the training tuples that were misclassified by M_i. TrAdaBoost follows this strategy for the target data. However, if a source data tuple is misclassified, TrAdaBoost reasons that the tuple is probably very different from the target data. It therefore *reduces* the weight of such tuples so that they will have less effect on the subsequent classifier. As a result, TrAdaBoost can learn an accurate classification model using only a small amount of new data and a large amount of old data, even when the new data alone are insufficient to train the model. Hence, in this way TrAdaBoost allows knowledge to be transferred from the old classifier to the new one.

A challenge with transfer learning is **negative transfer**, which occurs when the new classifier performs worse than if there had been no transfer at all. Work on how to avoid negative transfer is an area of future research. *Heterogeneous transfer learning*, which involves transferring knowledge from different feature spaces and multiple source domains, is another venue for further work. Much of the research on transfer learning to date has been on small-scale applications. The use of transfer learning on larger applications, such as social network analysis and video classification, is an area for further investigation.

9.8 Summary

- Unlike naïve Bayesian classification (which assumes class conditional independence), **Bayesian belief networks** allow class conditional independencies to be defined between subsets of variables. They provide a graphical model of causal relationships, on which learning can be performed. Trained Bayesian belief networks can be used for classification.

- **Backpropagation** is a neural network algorithm for classification that employs a method of gradient descent. It searches for a set of weights that can model the data so as to minimize the mean-squared distance between the network's class prediction and the actual class label of data tuples. Rules may be extracted from trained neural networks to help improve the interpretability of the learned network.
- A **support vector machine** is an algorithm for the classification of both linear and nonlinear data. It transforms the original data into a higher dimension, from where it can find a hyperplane for data separation using essential training tuples called **support vectors**.
- *Frequent patterns* reflect strong associations between attribute–value pairs (or items) in data and are used in **classification based on frequent patterns**. Approaches to this methodology include associative classification and discriminant frequent pattern–based classification. In **associative classification**, a classifier is built from association rules generated from frequent patterns. In **discriminative frequent pattern–based classification**, frequent patterns serve as combined features, which are considered in addition to single features when building a classification model.
- Decision tree classifiers, Bayesian classifiers, classification by backpropagation, support vector machines, and classification based on frequent patterns are all examples of **eager learners** in that they use training tuples to construct a generalization model and in this way are ready for classifying new tuples. This contrasts with **lazy learners** or **instance-based** methods of classification, such as nearest-neighbor classifiers and case-based reasoning classifiers, which store all of the training tuples in pattern space and wait until presented with a test tuple before performing generalization. Hence, lazy learners require efficient indexing techniques.
- In **genetic algorithms**, populations of rules "evolve" via operations of crossover and mutation until all rules within a population satisfy a specified threshold. **Rough set theory** can be used to approximately define classes that are not distinguishable based on the available attributes. **Fuzzy set** approaches replace "brittle" threshold cutoffs for continuous-valued attributes with membership degree functions.
- Binary classification schemes, such as support vector machines, can be adapted to handle **multiclass classification**. This involves constructing an ensemble of binary classifiers. Error-correcting codes can be used to increase the accuracy of the ensemble.
- **Semi-supervised classification** is useful when large amounts of unlabeled data exist. It builds a classifier using both labeled and unlabeled data. Examples of semi-supervised classification include *self-training* and *cotraining*.
- **Active learning** is a form of supervised learning that is also suitable for situations where data are abundant, yet the class labels are scarce or expensive to obtain. The learning algorithm can actively query a user (e.g., a human oracle) for labels. To keep costs down, the active learner aims to achieve high accuracy using as few labeled instances as possible.

- **Transfer learning** aims to extract the knowledge from one or more *source tasks* and apply the knowledge to a *target task*. TrAdaBoost is an example of the *instance-based approach* to transfer learning, which reweights some of the data from the source task and uses it to learn the target task, thereby requiring fewer labeled target-task tuples.

9.9 Exercises

9.1 The following table consists of training data from an employee database. The data have been generalized. For example, "31 ... 35" for *age* represents the age range of 31 to 35. For a given row entry, *count* represents the number of data tuples having the values for *department, status, age*, and *salary* given in that row.

department	*status*	*age*	*salary*	*count*
sales	senior	31 ... 35	46K ... 50K	30
sales	junior	26 ... 30	26K ... 30K	40
sales	junior	31 ... 35	31K ... 35K	40
systems	junior	21 ... 25	46K ... 50K	20
systems	senior	31 ... 35	66K ... 70K	5
systems	junior	26 ... 30	46K ... 50K	3
systems	senior	41 ... 45	66K ... 70K	3
marketing	senior	36 ... 40	46K ... 50K	10
marketing	junior	31 ... 35	41K ... 45K	4
secretary	senior	46 ... 50	36K ... 40K	4
secretary	junior	26 ... 30	26K ... 30K	6

Let *status* be the class-label attribute.

(a) Design a multilayer feed-forward neural network for the given data. Label the nodes in the input and output layers.

(b) Using the multilayer feed-forward neural network obtained in (a), show the weight values after one iteration of the backpropagation algorithm, given the training instance "*(sales, senior, 31 ... 35, 46K ... 50K)*". Indicate your initial weight values and biases and the learning rate used.

9.2 The *support vector machine* is a highly accurate classification method. However, SVM classifiers suffer from slow processing when training with a large set of data tuples. Discuss how to overcome this difficulty and develop a scalable SVM algorithm for efficient SVM classification in large data sets.

9.3 Compare and contrast *associative classification* and *discriminative frequent pattern–based classification.* Why is classification based on frequent patterns able to achieve higher classification accuracy in many cases than a classic decision tree method?

9.4 Compare the advantages and disadvantages of *eager* classification (e.g., decision tree, Bayesian, neural network) versus *lazy* classification (e.g., *k*-nearest neighbor, case-based reasoning).

9.5 Write an algorithm for *k-nearest-neighbor classification* given *k*, the nearest number of neighbors, and *n*, the number of attributes describing each tuple.

9.6 Briefly describe the classification processes using (a) *genetic algorithms*, (b) *rough sets*, and (c) *fuzzy sets*.

9.7 Example 9.3 showed a use of error-correcting codes for a *multiclass classification* problem having four classes.

(a) Suppose that, given an unknown tuple to label, the seven trained binary classifiers collectively output the codeword 0101110, which does not match a codeword for any of the four classes. Using error correction, what class label should be assigned to the tuple?

(b) Explain why using a 4-bit vector for the codewords is insufficient for error correction.

9.8 *Semi-supervised classification*, *active learning*, and *transfer learning* are useful for situations in which unlabeled data are abundant.

(a) Describe *semi-supervised classification*, *active learning*, and *transfer learning*. Elaborate on applications for which they are useful, as well as the challenges of these approaches to classification.

(b) Research and describe an approach to semi-supervised classification other than self-training and cotraining.

(c) Research and describe an approach to active learning other than pool-based learning.

(d) Research and describe an alternative approach to instance-based transfer learning.

9.10 Bibliographic Notes

For an introduction to Bayesian belief networks, see Darwiche [Dar10] and Heckerman [Hec96]. For a thorough presentation of probabilistic networks, see Pearl [Pea88] and Koller and Friedman [KF09]. Solutions for learning the belief network structure from training data given observable variables are proposed in Cooper and Herskovits [CH92]; Buntine [Bun94]; and Heckerman, Geiger, and Chickering [HGC95]. Algorithms for inference on belief networks can be found in Russell and Norvig [RN95] and Jensen [Jen96]. The method of gradient descent, described in Section 9.1.2, for training Bayesian belief networks, is given in Russell, Binder, Koller, and Kanazawa [RBKK95]. The example given in Figure 9.1 is adapted from Russell et al. [RBKK95].

Alternative strategies for learning belief networks with hidden variables include application of Dempster, Laird, and Rubin's [DLR77] EM (Expectation Maximization) algorithm (Lauritzen [Lau95]) and methods based on the minimum description length principle (Lam [Lam98]). Cooper [Coo90] showed that the general problem of inference in unconstrained belief networks is NP-hard. Limitations of belief networks, such as their large computational complexity (Laskey and Mahoney [LM97]), have prompted the exploration of hierarchical and composable Bayesian models (Pfeffer, Koller, Milch, and Takusagawa [PKMT99] and Xiang, Olesen, and Jensen [XOJ00]). These follow an object-oriented approach to knowledge representation. Fishelson and Geiger [FG02] present a Bayesian network for genetic linkage analysis.

The perceptron is a simple neural network, proposed in 1958 by Rosenblatt [Ros58], which became a landmark in early machine learning history. Its input units are randomly connected to a single layer of output linear threshold units. In 1969, Minsky and Papert [MP69] showed that perceptrons are incapable of learning concepts that are linearly inseparable. This limitation, as well as limitations on hardware at the time, dampened enthusiasm for research in computational neuronal modeling for nearly 20 years. Renewed interest was sparked following the presentation of the backpropagation algorithm in 1986 by Rumelhart, Hinton, and Williams [RHW86], as this algorithm can learn concepts that are linearly inseparable.

Since then, many variations of backpropagation have been proposed, involving, for example, alternative error functions (Hanson and Burr [HB87]); dynamic adjustment of the network topology (Mézard and Nadal [MN89]; Fahlman and Lebiere [FL90]; Le Cun, Denker, and Solla [LDS90]; and Harp, Samad, and Guha [HSG90]); and dynamic adjustment of the learning rate and momentum parameters (Jacobs [Jac88]). Other variations are discussed in Chauvin and Rumelhart [CR95]. Books on neural networks include Rumelhart and McClelland [RM86]; Hecht-Nielsen [HN90]; Hertz, Krogh, and Palmer [HKP91]; Chauvin and Rumelhart [CR95]; Bishop [Bis95]; Ripley [Rip96]; and Haykin [Hay99]. Many books on machine learning, such as Mitchell [Mit97] and Russell and Norvig [RN95], also contain good explanations of the backpropagation algorithm.

There are several techniques for extracting rules from neural networks, such as those found in these papers: [SN88, Gal93, TS93, Avn95, LSL95, CS96, LGT97]. The method of rule extraction described in Section 9.2.4 is based on Lu, Setiono, and Liu [LSL95]. Critiques of techniques for rule extraction from neural networks can be found in Craven and Shavlik [CS97]. Roy [Roy00] proposes that the theoretical foundations of neural networks are flawed with respect to assumptions made regarding how connectionist learning models the brain. An extensive survey of applications of neural networks in industry, business, and science is provided in Widrow, Rumelhart, and Lehr [WRL94].

Support Vector Machines (SVMs) grew out of early work by Vapnik and Chervonenkis on statistical learning theory [VC71]. The first paper on SVMs was presented by Boser, Guyon, and Vapnik [BGV92]. More detailed accounts can be found in books by Vapnik [Vap95, Vap98]. Good starting points include the tutorial on SVMs by Burges [Bur98], as well as textbook coverage by Haykin [Hay08], Kecman [Kec01], and Cristianini and Shawe-Taylor [CS-T00]. For methods for solving optimization problems, see Fletcher [Fle87] and Nocedal and Wright [NW99]. These references give additional details alluded to as "fancy math tricks" in our text, such as transformation of the problem to a Lagrangian formulation and subsequent solving using Karush-Kuhn-Tucker (KKT) conditions.

For the application of SVMs to regression, see Schölkopf, Bartlett, Smola, and Williamson [SBSW99] and Drucker, Burges, Kaufman, Smola, and Vapnik [DBK$^+$97]. Approaches to SVM for large data include the sequential minimal optimization algorithm by Platt [Pla98], decomposition approaches such as in Osuna, Freund, and Girosi [OFG97], and CB-SVM, a microclustering-based SVM algorithm for large data sets, by Yu, Yang, and Han [YYH03]. A library of software for support vector machines is provided by Chang and Lin at *www.csie.ntu.edu.tw/∼cjlin/libsvm/*, which supports multiclass classification.

Many algorithms have been proposed that adapt frequent pattern mining to the task of classification. Early studies on associative classification include the CBA algorithm, proposed in Liu, Hsu, and Ma [LHM98]. A classifier that uses *emerging patterns* (itemsets with support that varies significantly from one data set to another) is proposed in Dong and Li [DL99] and Li, Dong, and Ramamohanarao [LDR00]. CMAR is presented in Li, Han, and Pei [LHP01]. CPAR is presented in Yin and Han [YH03b]. Cong, Tan, Tung, and Xu describe RCBT, a method for mining top-k covering rule groups for classifying high-dimensional gene expression data with high accuracy [CTTX05].

Wang and Karypis [WK05] present HARMONY (Highest confidence classificAtion Rule Mining fOr iNstance-centric classifYing), which directly mines the final classification rule set with the aid of pruning strategies. Lent, Swami, and Widom [LSW97] propose the ARCS system regarding mining multidimensional association rules. It combines ideas from association rule mining, clustering, and image processing, and applies them to classification. Meretakis and Wüthrich [MW99] propose constructing a naïve Bayesian classifier by mining long itemsets. Veloso, Meira, and Zaki [VMZ06] propose an association rule–based classification method based on a lazy (noneager) learning approach, in which the computation is performed on a demand-driven basis.

Studies on discriminative frequent pattern–based classification were conducted by Cheng, Yan, Han, and Hsu [CYHH07] and Cheng, Yan, Han, and Yu [CYHY08]. The former work establishes a theoretical upper bound on the discriminative power of frequent patterns (based on either information gain [Qui86] or Fisher score [DHS01]), which can be used as a strategy for setting minimum support. The latter work describes the DDPMine algorithm, which is a direct approach to mining discriminative frequent patterns for classification in that it avoids generating the complete frequent pattern set. H. Kim, S. Kim, Weninger, et al. proposed an NDPMine algorithm that performs frequent and discriminative pattern–based classification by taking *repetitive* features into consideration [KKW$^+$10].

Nearest-neighbor classifiers were introduced in 1951 by Fix and Hodges [FH51]. A comprehensive collection of articles on nearest-neighbor classification can be found in Dasarathy [Das91]. Additional references can be found in many texts on classification, such as Duda, Hart, and Stork [DHS01] and James [Jam85], as well as articles by Cover and Hart [CH67] and Fukunaga and Hummels [FH87]. Their integration with attribute weighting and the pruning of noisy instances is described in Aha [Aha92]. The use of search trees to improve nearest-neighbor classification time is detailed in Friedman, Bentley, and Finkel [FBF77]. The partial distance method was proposed by researchers in vector quantization and compression. It is outlined in Gersho and Gray

[GG92]. The editing method for removing "useless" training tuples was first proposed by Hart [Har68].

The computational complexity of nearest-neighbor classifiers is described in Preparata and Shamos [PS85]. References on case-based reasoning include the texts by Riesbeck and Schank [RS89] and Kolodner [Kol93], as well as Leake [Lea96] and Aamodt and Plazas [AP94]. For a list of business applications, see Allen [All94]. Examples in medicine include CASEY by Koton [Kot88] and PROTOS by Bareiss, Porter, and Weir [BPW88], while Rissland and Ashley [RA87] is an example of CBR for law. CBR is available in several commercial software products. For texts on genetic algorithms, see Goldberg [Gol89], Michalewicz [Mic92], and Mitchell [Mit96].

Rough sets were introduced in Pawlak [Paw91]. Concise summaries of rough set theory in data mining include Ziarko [Zia91] and Cios, Pedrycz, and Swiniarski [CPS98]. Rough sets have been used for feature reduction and expert system design in many applications, including Ziarko [Zia91], Lenarcik and Piasta [LP97], and Swiniarski [Swi98]. Algorithms to reduce the computation intensity in finding reducts have been proposed in Skowron and Rauszer [SR92]. Fuzzy set theory was proposed by Zadeh [Zad65, Zad83]. Additional descriptions can be found in Yager and Zadeh [YZ94] and Kecman [Kec01].

Work on multiclass classification is described in Hastie and Tibshirani [HT98], Tax and Duin [TD02], and Allwein, Shapire, and Singer [ASS00]. Zhu [Zhu05] presents a comprehensive survey on semi-supervised classification. For additional references, see the book edited by Chapelle, Schölkopf, and Zien [CSZ06]. Dietterich and Bakiri [DB95] propose the use of error-correcting codes for multiclass classification. For a survey on active learning, see Settles [Set10]. Pan and Yang present a survey on transfer learning [PY10]. The TrAdaBoost boosting algorithm for transfer learning is given in Dai, Yang, Xue, and Yu [DYXY07].

10 Cluster Analysis: Basic Concepts and Methods

Imagine that you are the Director of Customer Relationships at *AllElectronics*, and you have five managers working for you. You would like to organize all the company's customers into five groups so that each group can be assigned to a different manager. Strategically, you would like that the customers in each group are as similar as possible. Moreover, two given customers having very different business patterns should not be placed in the same group. Your intention behind this business strategy is to develop customer relationship campaigns that specifically target each group, based on common features shared by the customers per group. What kind of data mining techniques can help you to accomplish this task?

Unlike in classification, the class label (or *group_ID*) of each customer is unknown. You need to *discover* these groupings. Given a large number of customers and many attributes describing customer profiles, it can be very costly or even infeasible to have a human study the data and manually come up with a way to partition the customers into strategic groups. You need a *clustering* tool to help.

Clustering is the process of grouping a set of data objects into multiple groups or *clusters* so that objects within a cluster have high similarity, but are very dissimilar to objects in other clusters. Dissimilarities and similarities are assessed based on the attribute values describing the objects and often involve distance measures.[1] Clustering as a data mining tool has its roots in many application areas such as biology, security, business intelligence, and Web search.

This chapter presents the basic concepts and methods of cluster analysis. In Section 10.1, we introduce the topic and study the requirements of clustering methods for massive amounts of data and various applications. You will learn several basic clustering techniques, organized into the following categories: *partitioning methods* (Section 10.2), *hierarchical methods* (Section 10.3), *density-based methods* (Section 10.4), and *grid-based methods* (Section 10.5). In Section 10.6, we briefly discuss how to evaluate

[1]Data similarity and dissimilarity are discussed in detail in Section 2.4. You may want to refer to that section for a quick review.

clustering methods. A discussion of advanced methods of clustering is reserved for Chapter 11.

10.1 Cluster Analysis

This section sets up the groundwork for studying cluster analysis. Section 10.1.1 defines cluster analysis and presents examples of where it is useful. In Section 10.1.2, you will learn aspects for comparing clustering methods, as well as requirements for clustering. An overview of basic clustering techniques is presented in Section 10.1.3.

10.1.1 What Is Cluster Analysis?

Cluster analysis or simply **clustering** is the process of partitioning a set of data objects (or observations) into subsets. Each subset is a **cluster**, such that objects in a cluster are similar to one another, yet dissimilar to objects in other clusters. The set of clusters resulting from a cluster analysis can be referred to as a **clustering**. In this context, different clustering methods may generate different clusterings on the same data set. The partitioning is not performed by humans, but by the clustering algorithm. Hence, clustering is useful in that it can lead to the discovery of previously unknown groups within the data.

Cluster analysis has been widely used in many applications such as business intelligence, image pattern recognition, Web search, biology, and security. In business intelligence, clustering can be used to organize a large number of customers into groups, where customers within a group share strong similar characteristics. This facilitates the development of business strategies for enhanced customer relationship management. Moreover, consider a consultant company with a large number of projects. To improve project management, clustering can be applied to partition projects into categories based on similarity so that project auditing and diagnosis (to improve project delivery and outcomes) can be conducted effectively.

In image recognition, clustering can be used to discover clusters or "subclasses" in handwritten character recognition systems. Suppose we have a data set of handwritten digits, where each digit is labeled as either 1, 2, 3, and so on. Note that there can be a large variance in the way in which people write the same digit. Take the number 2, for example. Some people may write it with a small circle at the left bottom part, while some others may not. We can use clustering to determine subclasses for "2," each of which represents a variation on the way in which 2 can be written. Using multiple models based on the subclasses can improve overall recognition accuracy.

Clustering has also found many applications in Web search. For example, a keyword search may often return a very large number of hits (i.e., pages relevant to the search) due to the extremely large number of web pages. Clustering can be used to organize the search results into groups and present the results in a concise and easily accessible way. Moreover, clustering techniques have been developed to cluster documents into topics, which are commonly used in information retrieval practice.

As a data mining function, cluster analysis can be used as a standalone tool to gain insight into the distribution of data, to observe the characteristics of each cluster, and to focus on a particular set of clusters for further analysis. Alternatively, it may serve as a preprocessing step for other algorithms, such as characterization, attribute subset selection, and classification, which would then operate on the detected clusters and the selected attributes or features.

Because a cluster is a collection of data objects that are similar to one another within the cluster and dissimilar to objects in other clusters, a cluster of data objects can be treated as an implicit class. In this sense, clustering is sometimes called **automatic classification**. Again, a critical difference here is that clustering can automatically find the groupings. This is a distinct advantage of cluster analysis.

Clustering is also called **data segmentation** in some applications because clustering partitions large data sets into groups according to their *similarity*. Clustering can also be used for **outlier detection**, where outliers (values that are "far away" from any cluster) may be more interesting than common cases. Applications of outlier detection include the detection of credit card fraud and the monitoring of criminal activities in electronic commerce. For example, exceptional cases in credit card transactions, such as very expensive and infrequent purchases, may be of interest as possible fraudulent activities. Outlier detection is the subject of Chapter 12.

Data clustering is under vigorous development. Contributing areas of research include data mining, statistics, machine learning, spatial database technology, information retrieval, Web search, biology, marketing, and many other application areas. Owing to the huge amounts of data collected in databases, cluster analysis has recently become a highly active topic in data mining research.

As a branch of statistics, cluster analysis has been extensively studied, with the main focus on *distance-based cluster analysis*. Cluster analysis tools based on *k*-means, *k*-medoids, and several other methods also have been built into many statistical analysis software packages or systems, such as S-Plus, SPSS, and SAS. In machine learning, recall that classification is known as supervised learning because the class label information is given, that is, the learning algorithm is supervised in that it is told the class membership of each training tuple. Clustering is known as **unsupervised learning** because the class label information is not present. For this reason, clustering is a form of **learning by observation**, rather than *learning by examples*. In data mining, efforts have focused on finding methods for efficient and effective cluster analysis in *large databases*. Active themes of research focus on the *scalability* of clustering methods, the effectiveness of methods for clustering *complex shapes* (e.g., nonconvex) and *types of data* (e.g., text, graphs, and images), *high-dimensional* clustering techniques (e.g., clustering objects with thousands of features), and methods for clustering *mixed numerical and nominal data* in large databases.

10.1.2 Requirements for Cluster Analysis

Clustering is a challenging research field. In this section, you will learn about the requirements for clustering as a data mining tool, as well as aspects that can be used for comparing clustering methods.

The following are typical requirements of clustering in data mining.

- **Scalability**: Many clustering algorithms work well on small data sets containing fewer than several hundred data objects; however, a large database may contain millions or even billions of objects, particularly in Web search scenarios. Clustering on only a sample of a given large data set may lead to biased results. Therefore, highly scalable clustering algorithms are needed.
- **Ability to deal with different types of attributes**: Many algorithms are designed to cluster numeric (interval-based) data. However, applications may require clustering other data types, such as binary, nominal (categorical), and ordinal data, or mixtures of these data types. Recently, more and more applications need clustering techniques for complex data types such as graphs, sequences, images, and documents.
- **Discovery of clusters with arbitrary shape**: Many clustering algorithms determine clusters based on Euclidean or Manhattan distance measures (Chapter 2). Algorithms based on such distance measures tend to find spherical clusters with similar size and density. However, a cluster could be of any shape. Consider sensors, for example, which are often deployed for environment surveillance. Cluster analysis on sensor readings can detect interesting phenomena. We may want to use clustering to find the frontier of a running forest fire, which is often not spherical. It is important to develop algorithms that can detect clusters of arbitrary shape.
- **Requirements for domain knowledge to determine input parameters**: Many clustering algorithms require users to provide domain knowledge in the form of input parameters such as the desired number of clusters. Consequently, the clustering results may be sensitive to such parameters. Parameters are often hard to determine, especially for high-dimensionality data sets and where users have yet to grasp a deep understanding of their data. Requiring the specification of domain knowledge not only burdens users, but also makes the quality of clustering difficult to control.
- **Ability to deal with noisy data**: Most real-world data sets contain outliers and/or missing, unknown, or erroneous data. Sensor readings, for example, are often noisy—some readings may be inaccurate due to the sensing mechanisms, and some readings may be erroneous due to interferences from surrounding transient objects. Clustering algorithms can be sensitive to such noise and may produce poor-quality clusters. Therefore, we need clustering methods that are robust to noise.
- **Incremental clustering and insensitivity to input order**: In many applications, incremental updates (representing newer data) may arrive at any time. Some clustering algorithms cannot incorporate incremental updates into existing clustering structures and, instead, have to recompute a new clustering from scratch. Clustering algorithms may also be sensitive to the input data order. That is, given a set of data objects, clustering algorithms may return dramatically different clusterings depending on the order in which the objects are presented. Incremental clustering algorithms and algorithms that are insensitive to the input order are needed.

- **Capability of clustering high-dimensionality data**: A data set can contain numerous dimensions or attributes. When clustering documents, for example, each keyword can be regarded as a dimension, and there are often thousands of keywords. Most clustering algorithms are good at handling low-dimensional data such as data sets involving only two or three dimensions. Finding clusters of data objects in a high-dimensional space is challenging, especially considering that such data can be very sparse and highly skewed.
- **Constraint-based clustering**: Real-world applications may need to perform clustering under various kinds of constraints. Suppose that your job is to choose the locations for a given number of new automatic teller machines (ATMs) in a city. To decide upon this, you may cluster households while considering constraints such as the city's rivers and highway networks and the types and number of customers per cluster. A challenging task is to find data groups with good clustering behavior that satisfy specified constraints.
- **Interpretability and usability**: Users want clustering results to be interpretable, comprehensible, and usable. That is, clustering may need to be tied in with specific semantic interpretations and applications. It is important to study how an application goal may influence the selection of clustering features and clustering methods.

The following are orthogonal aspects with which clustering methods can be compared:

- **The partitioning criteria**: In some methods, all the objects are partitioned so that no hierarchy exists among the clusters. That is, all the clusters are at the same level conceptually. Such a method is useful, for example, for partitioning customers into groups so that each group has its own manager. Alternatively, other methods partition data objects hierarchically, where clusters can be formed at different semantic levels. For example, in text mining, we may want to organize a corpus of documents into multiple general topics, such as "politics" and "sports," each of which may have subtopics, For instance, "football," "basketball," "baseball," and "hockey" can exist as subtopics of "sports." The latter four subtopics are at a lower level in the hierarchy than "sports."
- **Separation of clusters**: Some methods partition data objects into mutually exclusive clusters. When clustering customers into groups so that each group is taken care of by one manager, each customer may belong to only one group. In some other situations, the clusters may not be exclusive, that is, a data object may belong to more than one cluster. For example, when clustering documents into topics, a document may be related to multiple topics. Thus, the topics as clusters may not be exclusive.
- **Similarity measure**: Some methods determine the similarity between two objects by the distance between them. Such a distance can be defined on Euclidean space,

a road network, a vector space, or any other space. In other methods, the similarity may be defined by connectivity based on density or contiguity, and may not rely on the absolute distance between two objects. Similarity measures play a fundamental role in the design of clustering methods. While distance-based methods can often take advantage of optimization techniques, density- and continuity-based methods can often find clusters of arbitrary shape.

- **Clustering space**: Many clustering methods search for clusters within the entire given data space. These methods are useful for low-dimensionality data sets. With high-dimensional data, however, there can be many irrelevant attributes, which can make similarity measurements unreliable. Consequently, clusters found in the full space are often meaningless. It's often better to instead search for clusters within different subspaces of the same data set. *Subspace clustering* discovers clusters and subspaces (often of low dimensionality) that manifest object similarity.

To conclude, clustering algorithms have several requirements. These factors include scalability and the ability to deal with different types of attributes, noisy data, incremental updates, clusters of arbitrary shape, and constraints. Interpretability and usability are also important. In addition, clustering methods can differ with respect to the partitioning level, whether or not clusters are mutually exclusive, the similarity measures used, and whether or not subspace clustering is performed.

10.1.3 Overview of Basic Clustering Methods

There are many clustering algorithms in the literature. It is difficult to provide a crisp categorization of clustering methods because these categories may overlap so that a method may have features from several categories. Nevertheless, it is useful to present a relatively organized picture of clustering methods. In general, the major fundamental clustering methods can be classified into the following categories, which are discussed in the rest of this chapter.

Partitioning methods: Given a set of n objects, a partitioning method constructs k partitions of the data, where each partition represents a cluster and $k \leq n$. That is, it divides the data into k groups such that each group must contain at least one object. In other words, partitioning methods conduct one-level partitioning on data sets. The basic partitioning methods typically adopt *exclusive cluster separation.* That is, each object must belong to exactly one group. This requirement may be relaxed, for example, in fuzzy partitioning techniques. References to such techniques are given in the bibliographic notes (Section 10.9).

Most partitioning methods are distance-based. Given k, the number of partitions to construct, a partitioning method creates an initial partitioning. It then uses an **iterative relocation technique** that attempts to improve the partitioning by moving objects from one group to another. The general criterion of a good partitioning is that objects in the same cluster are "close" or related to each other, whereas objects in different clusters are "far apart" or very different. There are various kinds of other criteria for judging the quality of partitions. Traditional partitioning methods can be extended for subspace clustering, rather than searching the full data space. This is useful when there are many attributes and the data are sparse.

Achieving global optimality in partitioning-based clustering is often computationally prohibitive, potentially requiring an exhaustive enumeration of all the possible partitions. Instead, most applications adopt popular heuristic methods, such as greedy approaches like the *k-means* and the *k-medoids* algorithms, which progressively improve the clustering quality and approach a local optimum. These heuristic clustering methods work well for finding spherical-shaped clusters in small- to medium-size databases. To find clusters with complex shapes and for very large data sets, partitioning-based methods need to be extended. Partitioning-based clustering methods are studied in depth in Section 10.2.

Hierarchical methods: A hierarchical method creates a hierarchical decomposition of the given set of data objects. A hierarchical method can be classified as being either *agglomerative* or *divisive*, based on how the hierarchical decomposition is formed. The *agglomerative approach*, also called the *bottom-up* approach, starts with each object forming a separate group. It successively merges the objects or groups close to one another, until all the groups are merged into one (the topmost level of the hierarchy), or a termination condition holds. The *divisive approach*, also called the *top-down* approach, starts with all the objects in the same cluster. In each successive iteration, a cluster is split into smaller clusters, until eventually each object is in one cluster, or a termination condition holds.

Hierarchical clustering methods can be distance-based or density- and continuity-based. Various extensions of hierarchical methods consider clustering in subspaces as well.

Hierarchical methods suffer from the fact that once a step (merge or split) is done, it can never be undone. This rigidity is useful in that it leads to smaller computation costs by not having to worry about a combinatorial number of different choices. Such techniques cannot correct erroneous decisions; however, methods for improving the quality of hierarchical clustering have been proposed. Hierarchical clustering methods are studied in Section 10.3.

Density-based methods: Most partitioning methods cluster objects based on the distance between objects. Such methods can find only spherical-shaped clusters and encounter difficulty in discovering clusters of arbitrary shapes. Other clustering methods have been developed based on the notion of *density*. Their general idea is to continue growing a given cluster as long as the density (number of objects or data points) in the "neighborhood" exceeds some threshold. For example, for each data point within a given cluster, the neighborhood of a given radius has to contain at least a minimum number of points. Such a method can be used to filter out noise or outliers and discover clusters of arbitrary shape.

Density-based methods can divide a set of objects into multiple exclusive clusters, or a hierarchy of clusters. Typically, density-based methods consider exclusive clusters only, and do not consider fuzzy clusters. Moreover, density-based methods can be extended from full space to subspace clustering. Density-based clustering methods are studied in Section 10.4.

Grid-based methods: Grid-based methods quantize the object space into a finite number of cells that form a grid structure. All the clustering operations are performed on the grid structure (i.e., on the quantized space). The main advantage of this approach is its fast processing time, which is typically independent of the number of data objects and dependent only on the number of cells in each dimension in the quantized space.

Using grids is often an efficient approach to many spatial data mining problems, including clustering. Therefore, grid-based methods can be integrated with other clustering methods such as density-based methods and hierarchical methods. Grid-based clustering is studied in Section 10.5.

These methods are briefly summarized in Figure 10.1. Some clustering algorithms integrate the ideas of several clustering methods, so that it is sometimes difficult to classify a given algorithm as uniquely belonging to only one clustering method category. Furthermore, some applications may have clustering criteria that require the integration of several clustering techniques.

In the following sections, we examine each clustering method in detail. Advanced clustering methods and related issues are discussed in Chapter 11. In general, the notation used is as follows. Let D be a data set of n objects to be clustered. An object is described by d variables, where each variable is also called an attribute or a dimension,

Method	**General Characteristics**
Partitioning methods	– Find mutually exclusive clusters of spherical shape – Distance-based – May use mean or medoid (etc.) to represent cluster center – Effective for small- to medium-size data sets
Hierarchical methods	– Clustering is a hierarchical decomposition (i.e., multiple levels) – Cannot correct erroneous merges or splits – May incorporate other techniques like microclustering or consider object "linkages"
Density-based methods	– Can find arbitrarily shaped clusters – Clusters are dense regions of objects in space that are separated by low-density regions – Cluster density: Each point must have a minimum number of points within its "neighborhood" – May filter out outliers
Grid-based methods	– Use a multiresolution grid data structure – Fast processing time (typically independent of the number of data objects, yet dependent on grid size)

Figure 10.1 Overview of clustering methods discussed in this chapter. Note that some algorithms may combine various methods.

and therefore may also be referred to as a *point* in a d-dimensional object space. Objects are represented in bold italic font (e.g., $\boldsymbol{p}$).

10.2 Partitioning Methods

The simplest and most fundamental version of cluster analysis is partitioning, which organizes the objects of a set into several exclusive groups or clusters. To keep the problem specification concise, we can assume that the number of clusters is given as background knowledge. This parameter is the starting point for partitioning methods.

Formally, given a data set, D, of n objects, and k, the number of clusters to form, a **partitioning algorithm** organizes the objects into k partitions ($k \leq n$), where each partition represents a cluster. The clusters are formed to optimize an objective partitioning criterion, such as a dissimilarity function based on distance, so that the objects within a cluster are "similar" to one another and "dissimilar" to objects in other clusters in terms of the data set attributes.

In this section you will learn the most well-known and commonly used partitioning methods—k-means (Section 10.2.1) and k-medoids (Section 10.2.2). You will also learn several variations of these classic partitioning methods and how they can be scaled up to handle large data sets.

10.2.1 *k*-Means: A Centroid-Based Technique

Suppose a data set, D, contains n objects in Euclidean space. Partitioning methods distribute the objects in D into k clusters, $C_1, \ldots, C_k$, that is, $C_i \subset D$ and $C_i \cap C_j = \emptyset$ for $(1 \leq i, j \leq k)$. An objective function is used to assess the partitioning quality so that objects within a cluster are similar to one another but dissimilar to objects in other clusters. This is, the objective function aims for high intracluster similarity and low intercluster similarity.

A centroid-based partitioning technique uses the *centroid* of a cluster, C_i, to represent that cluster. Conceptually, the centroid of a cluster is its center point. The centroid can be defined in various ways such as by the mean or medoid of the objects (or points) assigned to the cluster. The difference between an object $\boldsymbol{p} \in C_i$ and $\boldsymbol{c_i}$, the representative of the cluster, is measured by $dist(\boldsymbol{p}, \boldsymbol{c_i})$, where $dist(\boldsymbol{x}, \boldsymbol{y})$ is the Euclidean distance between two points $\boldsymbol{x}$ and $\boldsymbol{y}$. The quality of cluster C_i can be measured by the **within-cluster variation**, which is the sum of *squared error* between all objects in C_i and the centroid $\boldsymbol{c_i}$, defined as

$$E = \sum_{i=1}^{k} \sum_{p \in C_i} dist(\boldsymbol{p}, \boldsymbol{c_i})^2, \tag{10.1}$$

where E is the sum of the squared error for all objects in the data set; $\boldsymbol{p}$ is the point in space representing a given object; and $\boldsymbol{c_i}$ is the centroid of cluster C_i (both $\boldsymbol{p}$ and $\boldsymbol{c_i}$ are multidimensional). In other words, for each object in each cluster, the distance from the object to its cluster center is squared, and the distances are summed. This objective function tries to make the resulting k clusters as compact and as separate as possible.

Optimizing the within-cluster variation is computationally challenging. In the worst case, we would have to enumerate a number of possible partitionings that are exponential to the number of clusters, and check the within-cluster variation values. It has been shown that the problem is NP-hard in general Euclidean space even for two clusters (i.e., $k = 2$). Moreover, the problem is NP-hard for a general number of clusters k even in the 2-D Euclidean space. If the number of clusters k and the dimensionality of the space d are fixed, the problem can be solved in time $O(n^{dk+1} \log n)$, where n is the number of objects. To overcome the prohibitive computational cost for the exact solution, greedy approaches are often used in practice. A prime example is the k-means algorithm, which is simple and commonly used.

"How does the k-*means algorithm work?"* The k-means algorithm defines the centroid of a cluster as the mean value of the points within the cluster. It proceeds as follows. First, it randomly selects k of the objects in D, each of which initially represents a cluster mean or center. For each of the remaining objects, an object is assigned to the cluster to which it is the most similar, based on the Euclidean distance between the object and the cluster mean. The k-means algorithm then iteratively improves the within-cluster variation. For each cluster, it computes the new mean using the objects assigned to the cluster in the previous iteration. All the objects are then reassigned using the updated means as the new cluster centers. The iterations continue until the assignment is stable, that is, the clusters formed in the current round are the same as those formed in the previous round. The k-means procedure is summarized in Figure 10.2.

Algorithm: *k*-means. The k-means algorithm for partitioning, where each cluster's center is represented by the mean value of the objects in the cluster.

Input:

- k: the number of clusters,
- D: a data set containing n objects.

Output: A set of k clusters.

Method:

```
(1) arbitrarily choose $k$ objects from $D$ as the initial cluster centers;
(2) repeat
(3)       (re)assign each object to the cluster to which the object is the most similar,
                based on the mean value of the objects in the cluster;
(4)       update the cluster means, that is, calculate the mean value of the objects for
                each cluster;
(5) until no change;
```

Figure 10.2 The k-means partitioning algorithm.

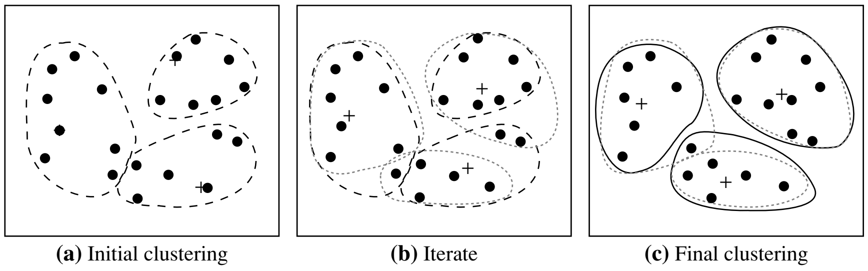


Figure 10.3 Clustering of a set of objects using the k-means method; for (b) update cluster centers and reassign objects accordingly (the mean of each cluster is marked by a $+$).

Example 10.1 **Clustering by k-means partitioning.** Consider a set of objects located in 2-D space, as depicted in Figure 10.3(a). Let $k = 3$, that is, the user would like the objects to be partitioned into three clusters.

According to the algorithm in Figure 10.2, we arbitrarily choose three objects as the three initial cluster centers, where cluster centers are marked by a $+$. Each object is assigned to a cluster based on the cluster center to which it is the nearest. Such a distribution forms silhouettes encircled by dotted curves, as shown in Figure 10.3(a).

Next, the cluster centers are updated. That is, the mean value of each cluster is recalculated based on the current objects in the cluster. Using the new cluster centers, the objects are redistributed to the clusters based on which cluster center is the nearest. Such a redistribution forms new silhouettes encircled by dashed curves, as shown in Figure 10.3(b).

This process iterates, leading to Figure 10.3(c). The process of iteratively reassigning objects to clusters to improve the partitioning is referred to as *iterative relocation*. Eventually, no reassignment of the objects in any cluster occurs and so the process terminates. The resulting clusters are returned by the clustering process. ■

The k-means method is not guaranteed to converge to the global optimum and often terminates at a local optimum. The results may depend on the initial random selection of cluster centers. (You will be asked to give an example to show this as an exercise.) To obtain good results in practice, it is common to run the k-means algorithm multiple times with different initial cluster centers.

The time complexity of the k-means algorithm is $O(nkt)$, where n is the total number of objects, k is the number of clusters, and t is the number of iterations. Normally, $k \ll n$ and $t \ll n$. Therefore, the method is relatively scalable and efficient in processing large data sets.

There are several variants of the k-means method. These can differ in the selection of the initial k-means, the calculation of dissimilarity, and the strategies for calculating cluster means.

The *k*-means method can be applied only when the mean of a set of objects is defined. This may not be the case in some applications such as when data with nominal attributes are involved. The ***k*-modes method** is a variant of *k*-means, which extends the *k*-means paradigm to cluster nominal data by replacing the means of clusters with modes. It uses new dissimilarity measures to deal with nominal objects and a frequency-based method to update modes of clusters. The *k*-means and the *k*-modes methods can be integrated to cluster data with mixed numeric and nominal values.

The necessity for users to specify *k*, the number of clusters, in advance can be seen as a disadvantage. There have been studies on how to overcome this difficulty, however, such as by providing an approximate range of *k* values, and then using an analytical technique to determine the best *k* by comparing the clustering results obtained for the different *k* values. The *k*-means method is not suitable for discovering clusters with nonconvex shapes or clusters of very different size. Moreover, it is sensitive to noise and outlier data points because a small number of such data can substantially influence the mean value.

"How can we make the k*-means algorithm more scalable?"* One approach to making the *k*-means method more efficient on large data sets is to use a good-sized set of samples in clustering. Another is to employ a filtering approach that uses a spatial hierarchical data index to save costs when computing means. A third approach explores the microclustering idea, which first groups nearby objects into "microclusters" and then performs *k*-means clustering on the microclusters. Microclustering is further discussed in Section 10.3.

10.2.2 *k*-Medoids: A Representative Object-Based Technique

The *k*-means algorithm is sensitive to outliers because such objects are far away from the majority of the data, and thus, when assigned to a cluster, they can dramatically distort the mean value of the cluster. This inadvertently affects the assignment of other objects to clusters. This effect is particularly exacerbated due to the use of the *squared*-error function of Eq. (10.1), as observed in Example 10.2.

Example 10.2 **A drawback of *k*-means.** Consider six points in 1-D space having the values $1,2,3,8,9,10$, and 25, respectively. Intuitively, by visual inspection we may imagine the points partitioned into the clusters $\{1,2,3\}$ and $\{8,9,10\}$, where point 25 is excluded because it appears to be an outlier. How would *k*-means partition the values? If we apply *k*-means using $k=2$ and Eq. (10.1), the partitioning $\{\{1,2,3\},\{8,9,10,25\}\}$ has the within-cluster variation

$$(1-2)^2+(2-2)^2+(3-2)^2+(8-13)^2+(9-13)^2+(10-13)^2+(25-13)^2=196,$$

given that the mean of cluster $\{1,2,3\}$ is 2 and the mean of $\{8,9,10,25\}$ is 13. Compare this to the partitioning $\{\{1,2,3,8\},\{9,10,25\}\}$, for which *k*-means computes the within-cluster variation as

$$(1-3.5)^2+(2-3.5)^2+(3-3.5)^2+(8-3.5)^2+(9-14.67)^2$$
$$+(10-14.67)^2+(25-14.67)^2=189.67,$$

given that 3.5 is the mean of cluster $\{1,2,3,8\}$ and 14.67 is the mean of cluster $\{9,10,25\}$. The latter partitioning has the lowest within-cluster variation; therefore, the k-means method assigns the value 8 to a cluster different from that containing 9 and 10 due to the outlier point 25. Moreover, the center of the second cluster, 14.67, is substantially far from all the members in the cluster. ■

"How can we modify the k-means algorithm to diminish such sensitivity to outliers?" Instead of taking the mean value of the objects in a cluster as a reference point, we can pick actual objects to represent the clusters, using one representative object per cluster. Each remaining object is assigned to the cluster of which the representative object is the most similar. The partitioning method is then performed based on the principle of minimizing the sum of the dissimilarities between each object $\boldsymbol{p}$ and its corresponding representative object. That is, an **absolute-error criterion** is used, defined as

$$E=\sum_{i=1}^{k}\sum_{\boldsymbol{p}\in C_i} dist(\boldsymbol{p},\boldsymbol{o}_i), \tag{10.2}$$

where E is the sum of the absolute error for all objects $\boldsymbol{p}$ in the data set, and $\boldsymbol{o_i}$ is the representative object of C_i. This is the basis for the ***k*-medoids method**, which groups n objects into k clusters by minimizing the absolute error (Eq. 10.2).

When $k=1$, we can find the exact median in $O(n^2)$ time. However, when k is a general positive number, the k-medoid problem is NP-hard.

The **Partitioning Around Medoids (PAM)** algorithm (see Figure 10.5 later) is a popular realization of k-medoids clustering. It tackles the problem in an iterative, greedy way. Like the k-means algorithm, the initial representative objects (called seeds) are chosen arbitrarily. We consider whether replacing a representative object by a nonrepresentative object would improve the clustering quality. All the possible replacements are tried out. The iterative process of replacing representative objects by other objects continues until the quality of the resulting clustering cannot be improved by any replacement. This quality is measured by a cost function of the average dissimilarity between an object and the representative object of its cluster.

Specifically, let $\boldsymbol{o}_1,\ldots,\boldsymbol{o_k}$ be the current set of representative objects (i.e., medoids). To determine whether a nonrepresentative object, denoted by $\boldsymbol{o_{random}}$, is a good replacement for a current medoid $\boldsymbol{o_j}$ $(1\le j\le k)$, we calculate the distance from every object $\boldsymbol{p}$ to the closest object in the set $\{\boldsymbol{o}_1,\ldots,\boldsymbol{o}_{j-1},\boldsymbol{o_{random}},\boldsymbol{o}_{j+1},\ldots,\boldsymbol{o_k}\}$, and use the distance to update the cost function. The reassignments of objects to $\{\boldsymbol{o}_1,\ldots,\boldsymbol{o}_{j-1},\boldsymbol{o_{random}},\boldsymbol{o}_{j+1},\ldots,\boldsymbol{o_k}\}$ are simple. Suppose object $\boldsymbol{p}$ is currently assigned to a cluster represented by medoid $\boldsymbol{o_j}$ (Figure 10.4a or b). Do we need to reassign $\boldsymbol{p}$ to a different cluster if $\boldsymbol{o_j}$ is being replaced by $\boldsymbol{o_{random}}$? Object $\boldsymbol{p}$ needs to be reassigned to either $\boldsymbol{o_{random}}$ or some other cluster represented by $\boldsymbol{o_i}$ $(i\neq j)$, whichever is the closest. For example, in Figure 10.4(a), $\boldsymbol{p}$ is closest to $\boldsymbol{o_i}$ and therefore is reassigned to $\boldsymbol{o_i}$. In Figure 10.4(b), however, $\boldsymbol{p}$ is closest to $\boldsymbol{o_{random}}$ and so is reassigned to $\boldsymbol{o_{random}}$. What if, instead, $\boldsymbol{p}$ is currently assigned to a cluster represented by some other object $\boldsymbol{o_i}$, $i\neq j$?

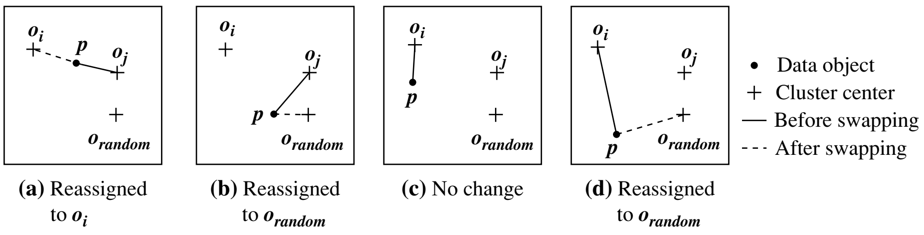


Figure 10.4 Four cases of the cost function for *k*-medoids clustering.

Object $\boldsymbol{o}$ remains assigned to the cluster represented by $\boldsymbol{o_i}$ as long as $\boldsymbol{o}$ is still closer to $\boldsymbol{o_i}$ than to $\boldsymbol{o_{random}}$ (Figure 10.4c). Otherwise, $\boldsymbol{o}$ is reassigned to $\boldsymbol{o_{random}}$ (Figure 10.4d).

Each time a reassignment occurs, a difference in absolute error, E, is contributed to the cost function. Therefore, the cost function calculates the *difference* in absolute-error value if a current representative object is replaced by a nonrepresentative object. The total cost of swapping is the sum of costs incurred by all nonrepresentative objects. If the total cost is negative, then $\boldsymbol{o_j}$ is replaced or swapped with $\boldsymbol{o_{random}}$ because the actual absolute-error E is reduced. If the total cost is positive, the current representative object, $\boldsymbol{o_j}$, is considered acceptable, and nothing is changed in the iteration.

"Which method is more robust—k-means or k-medoids?" The *k*-medoids method is more robust than *k*-means in the presence of noise and outliers because a medoid is less influenced by outliers or other extreme values than a mean. However, the complexity of each iteration in the *k*-medoids algorithm is $O(k(n-k)^2)$. For large values of n and k, such computation becomes very costly, and much more costly than the *k*-means method. Both methods require the user to specify k, the number of clusters.

"How can we scale up the k-medoids method?" A typical *k*-medoids partitioning algorithm like PAM (Figure 10.5) works effectively for small data sets, but does not scale well for large data sets. To deal with larger data sets, a *sampling*-based method called **CLARA** (**Clustering LARge Applications**) can be used. Instead of taking the whole data set into consideration, CLARA uses a random sample of the data set. The PAM algorithm is then applied to compute the best medoids from the sample. Ideally, the sample should closely represent the original data set. In many cases, a large sample works well if it is created so that each object has equal probability of being selected into the sample. The representative objects (medoids) chosen will likely be similar to those that would have been chosen from the whole data set. CLARA builds clusterings from multiple random samples and returns the best clustering as the output. The complexity of computing the medoids on a random sample is $O(ks^2 + k(n-k))$, where s is the size of the sample, k is the number of clusters, and n is the total number of objects. CLARA can deal with larger data sets than PAM.

The effectiveness of CLARA depends on the sample size. Notice that PAM searches for the best *k*-medoids among a given data set, whereas CLARA searches for the best *k*-medoids among the *selected sample* of the data set. CLARA cannot find a good clustering if any of the best sampled medoids is far from the best *k*-medoids. If an object

Algorithm: ***k*-medoids.** PAM, a *k*-medoids algorithm for partitioning based on medoid or central objects.

Input:

- *k*: the number of clusters,
- *D*: a data set containing *n* objects.

Output: A set of *k* clusters.

Method:

```
(1)  arbitrarily choose $k$ objects in $D$ as the initial representative objects or seeds;
(2)  repeat
(3)      assign each remaining object to the cluster with the nearest representative object;
(4)      randomly select a nonrepresentative object, $o_{random}$;
(5)      compute the total cost, $S$, of swapping representative object, $o_j$, with $o_{random}$;
(6)      if $S < 0$ then swap $o_j$ with $o_{random}$ to form the new set of $k$ representative objects;
(7)  until no change;
```

Figure 10.5 PAM, a *k*-medoids partitioning algorithm.

is one of the best *k*-medoids but is not selected during sampling, CLARA will never find the best clustering. (You will be asked to provide an example demonstrating this as an exercise.)

"*How might we improve the quality and scalability of CLARA?*" Recall that when searching for better medoids, PAM examines every object in the data set against every current medoid, whereas CLARA confines the candidate medoids to only a random sample of the data set. A randomized algorithm called **CLARANS** (Clustering Large Applications based upon RANdomized Search) presents a trade-off between the cost and the effectiveness of using samples to obtain clustering.

First, it randomly selects *k* objects in the data set as the current medoids. It then randomly selects a current medoid $\boldsymbol{x}$ and an object $\boldsymbol{y}$ that is not one of the current medoids. Can replacing $\boldsymbol{x}$ by $\boldsymbol{y}$ improve the absolute-error criterion? If yes, the replacement is made. CLARANS conducts such a randomized search *l* times. The set of the current medoids after the *l* steps is considered a local optimum. CLARANS repeats this randomized process *m* times and returns the best local optimal as the final result.

10.3 Hierarchical Methods

While partitioning methods meet the basic clustering requirement of organizing a set of objects into a number of exclusive groups, in some situations we may want to partition our data into groups at different levels such as in a hierarchy. A **hierarchical clustering method** works by grouping data objects into a hierarchy or "tree" of clusters.

Representing data objects in the form of a hierarchy is useful for data summarization and visualization. For example, as the manager of human resources at *AllElectronics*, you may organize your employees into major groups such as executives, managers, and staff. You can further partition these groups into smaller subgroups. For instance, the general group of staff can be further divided into subgroups of senior officers, officers, and trainees. All these groups form a hierarchy. We can easily summarize or characterize the data that are organized into a hierarchy, which can be used to find, say, the average salary of managers and of officers.

Consider handwritten character recognition as another example. A set of handwriting samples may be first partitioned into general groups where each group corresponds to a unique character. Some groups can be further partitioned into subgroups since a character may be written in multiple substantially different ways. If necessary, the hierarchical partitioning can be continued recursively until a desired granularity is reached.

In the previous examples, although we partitioned the data hierarchically, we did not assume that the data have a hierarchical structure (e.g., managers are at the same level in our *AllElectronics* hierarchy as staff). Our use of a hierarchy here is just to summarize and represent the underlying data in a compressed way. Such a hierarchy is particularly useful for data visualization.

Alternatively, in some applications we may believe that the data bear an underlying hierarchical structure that we want to discover. For example, hierarchical clustering may uncover a hierarchy for *AllElectronics* employees structured on, say, salary. In the study of evolution, hierarchical clustering may group animals according to their biological features to uncover evolutionary paths, which are a hierarchy of species. As another example, grouping configurations of a strategic game (e.g., chess or checkers) in a hierarchical way may help to develop game strategies that can be used to train players.

In this section, you will study hierarchical clustering methods. Section 10.3.1 begins with a discussion of agglomerative versus divisive hierarchical clustering, which organize objects into a hierarchy using a bottom-up or top-down strategy, respectively. Agglomerative methods start with individual objects as clusters, which are iteratively merged to form larger clusters. Conversely, divisive methods initially let all the given objects form one cluster, which they iteratively split into smaller clusters.

Hierarchical clustering methods can encounter difficulties regarding the selection of merge or split points. Such a decision is critical, because once a group of objects is merged or split, the process at the next step will operate on the newly generated clusters. It will neither undo what was done previously, nor perform object swapping between clusters. Thus, merge or split decisions, if not well chosen, may lead to low-quality clusters. Moreover, the methods do not scale well because each decision of merge or split needs to examine and evaluate many objects or clusters.

A promising direction for improving the clustering quality of hierarchical methods is to integrate hierarchical clustering with other clustering techniques, resulting in **multiple-phase** (or **multiphase**) **clustering**. We introduce two such methods, namely BIRCH and Chameleon. BIRCH (Section 10.3.3) begins by partitioning objects hierarchically using tree structures, where the leaf or low-level nonleaf nodes can be viewed as "microclusters" depending on the resolution scale. It then applies other clustering algorithms to perform macroclustering on the microclusters. Chameleon (Section 10.3.4) explores dynamic modeling in hierarchical clustering.

There are several orthogonal ways to categorize hierarchical clustering methods. For instance, they may be categorized into *algorithmic* methods, *probabilistic* methods, and *Bayesian* methods. Agglomerative, divisive, and multiphase methods are *algorithmic*, meaning they consider data objects as deterministic and compute clusters according to the deterministic distances between objects. Probabilistic methods use probabilistic models to capture clusters and measure the quality of clusters by the fitness of models. We discuss probabilistic hierarchical clustering in Section 10.3.5. *Bayesian methods* compute a distribution of possible clusterings. That is, instead of outputting a single deterministic clustering over a data set, they return a group of clustering structures and their probabilities, conditional on the given data. Bayesian methods are considered an advanced topic and are not discussed in this book.

10.3.1 Agglomerative versus Divisive Hierarchical Clustering

A hierarchical clustering method can be either *agglomerative* or *divisive*, depending on whether the hierarchical decomposition is formed in a bottom-up (merging) or top-down (splitting) fashion. Let's have a closer look at these strategies.

An **agglomerative hierarchical clustering method** uses a bottom-up strategy. It typically starts by letting each object form its own cluster and iteratively merges clusters into larger and larger clusters, until all the objects are in a single cluster or certain termination conditions are satisfied. The single cluster becomes the hierarchy's root. For the merging step, it finds the two clusters that are closest to each other (according to some similarity measure), and combines the two to form one cluster. Because two clusters are merged per iteration, where each cluster contains at least one object, an agglomerative method requires at most n iterations.

A **divisive hierarchical clustering method** employs a top-down strategy. It starts by placing all objects in one cluster, which is the hierarchy's root. It then divides the root cluster into several smaller subclusters, and recursively partitions those clusters into smaller ones. The partitioning process continues until each cluster at the lowest level is coherent enough—either containing only one object, or the objects within a cluster are sufficiently similar to each other.

In either agglomerative or divisive hierarchical clustering, a user can specify the desired number of clusters as a termination condition.

Example 10.3 **Agglomerative versus divisive hierarchical clustering.** Figure 10.6 shows the application of **AGNES** (AGglomerative NESting), an agglomerative hierarchical clustering method, and **DIANA** (DIvisive ANAlysis), a divisive hierarchical clustering method, on a data set of five objects, $\{\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \boldsymbol{d}, \boldsymbol{e}\}$. Initially, AGNES, the agglomerative method, places each object into a cluster of its own. The clusters are then merged step-by-step according to some criterion. For example, clusters C_1 and C_2 may be merged if an object in C_1 and an object in C_2 form the minimum Euclidean distance between any two objects from

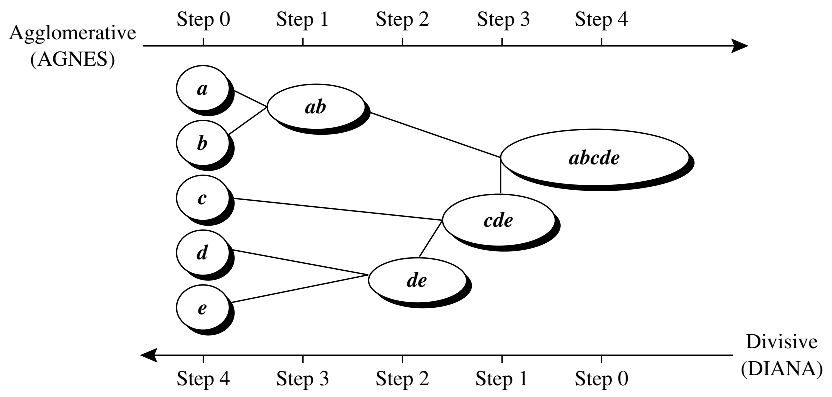


Figure 10.6 Agglomerative and divisive hierarchical clustering on data objects $\{a, b, c, d, e\}$.

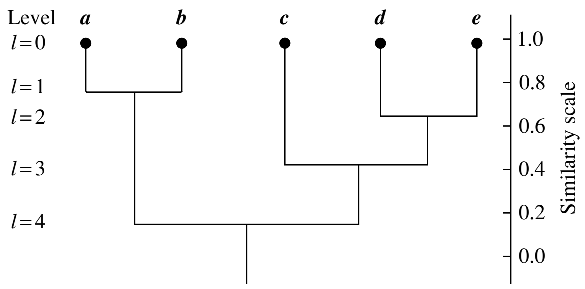


Figure 10.7 Dendrogram representation for hierarchical clustering of data objects $\{a, b, c, d, e\}$.

different clusters. This is a **single-linkage** approach in that each cluster is represented by all the objects in the cluster, and the similarity between two clusters is measured by the similarity of the *closest* pair of data points belonging to different clusters. The cluster-merging process repeats until all the objects are eventually merged to form one cluster.

DIANA, the divisive method, proceeds in the contrasting way. All the objects are used to form one initial cluster. The cluster is split according to some principle such as the maximum Euclidean distance between the closest neighboring objects in the cluster. The cluster-splitting process repeats until, eventually, each new cluster contains only a single object. ■

A tree structure called a **dendrogram** is commonly used to represent the process of hierarchical clustering. It shows how objects are grouped together (in an agglomerative method) or partitioned (in a divisive method) step-by-step. Figure 10.7 shows a dendrogram for the five objects presented in Figure 10.6, where $l = 0$ shows the five objects as singleton clusters at level 0. At $l = 1$, objects a and b are grouped together to form the first cluster, and they stay together at all subsequent levels. We can also use a vertical axis to show the similarity scale between clusters. For example, when the similarity of two groups of objects, $\{\boldsymbol{a}, \boldsymbol{b}\}$ and $\{\boldsymbol{c}, \boldsymbol{d}, \boldsymbol{e}\}$, is roughly 0.16, they are merged together to form a single cluster.

A challenge with divisive methods is how to partition a large cluster into several smaller ones. For example, there are $2^{n-1} - 1$ possible ways to partition a set of n objects into two exclusive subsets, where n is the number of objects. When n is large, it is computationally prohibitive to examine all possibilities. Consequently, a divisive method typically uses heuristics in partitioning, which can lead to inaccurate results. For the sake of efficiency, divisive methods typically do not backtrack on partitioning decisions that have been made. Once a cluster is partitioned, any alternative partitioning of this cluster will not be considered again. Due to the challenges in divisive methods, there are many more agglomerative methods than divisive methods.

10.3.2 Distance Measures in Algorithmic Methods

Whether using an agglomerative method or a divisive method, a core need is to measure the distance between two clusters, where each cluster is generally a set of objects.

Four widely used measures for distance between clusters are as follows, where $|\boldsymbol{p} - \boldsymbol{p}'|$ is the distance between two objects or points, $\boldsymbol{p}$ and $\boldsymbol{p}'$; $\boldsymbol{m_i}$ is the mean for cluster, C_i; and n_i is the number of objects in C_i. They are also known as *linkage measures.*

$$\textbf{Minimum distance:}\quad dist_{min}(C_i, C_j) = \min_{\boldsymbol{p}\in C_i, \boldsymbol{p}'\in C_j} \{|\boldsymbol{p} - \boldsymbol{p}'|\} \tag{10.3}$$

$$\textbf{Maximum distance:}\quad dist_{max}(C_i, C_j) = \max_{\boldsymbol{p}\in C_i, \boldsymbol{p}'\in C_j} \{|\boldsymbol{p} - \boldsymbol{p}'|\} \tag{10.4}$$

$$\textbf{Mean distance:}\quad dist_{mean}(C_i, C_j) = |\boldsymbol{m_i} - \boldsymbol{m_j}| \tag{10.5}$$

$$\textbf{Average distance:}\quad dist_{avg}(C_i, C_j) = \frac{1}{n_i n_j} \sum_{\boldsymbol{p}\in C_i, \boldsymbol{p}'\in C_j} |\boldsymbol{p} - \boldsymbol{p}'| \tag{10.6}$$

When an algorithm uses the *minimum distance*, $d_{min}(C_i, C_j)$, to measure the distance between clusters, it is sometimes called a **nearest-neighbor clustering algorithm**. Moreover, if the clustering process is terminated when the distance between nearest clusters exceeds a user-defined threshold, it is called a **single-linkage algorithm**. If we view the data points as nodes of a graph, with edges forming a path between the nodes in a cluster, then the merging of two clusters, C_i and C_j, corresponds to adding an edge between the nearest pair of nodes in C_i and C_j. Because edges linking clusters always go between distinct clusters, the resulting graph will generate a tree. Thus, an agglomerative hierarchical clustering algorithm that uses the minimum distance measure is also called a

minimal spanning tree algorithm, where a spanning tree of a graph is a tree that connects all vertices, and a minimal spanning tree is the one with the least sum of edge weights.

When an algorithm uses the *maximum distance*, $d_{max}(C_i, C_j)$, to measure the distance between clusters, it is sometimes called a **farthest-neighbor clustering algorithm**. If the clustering process is terminated when the maximum distance between nearest clusters exceeds a user-defined threshold, it is called a **complete-linkage algorithm**. By viewing data points as nodes of a graph, with edges linking nodes, we can think of each cluster as a *complete* subgraph, that is, with edges connecting all the nodes in the clusters. The distance between two clusters is determined by the most distant nodes in the two clusters. Farthest-neighbor algorithms tend to minimize the increase in diameter of the clusters at each iteration. If the true clusters are rather compact and approximately equal size, the method will produce high-quality clusters. Otherwise, the clusters produced can be meaningless.

The previous minimum and maximum measures represent two extremes in measuring the distance between clusters. They tend to be overly sensitive to outliers or noisy data. The use of *mean* or *average distance* is a compromise between the minimum and maximum distances and overcomes the outlier sensitivity problem. Whereas the *mean distance* is the simplest to compute, the *average distance* is advantageous in that it can handle categoric as well as numeric data. The computation of the mean vector for categoric data can be difficult or impossible to define.

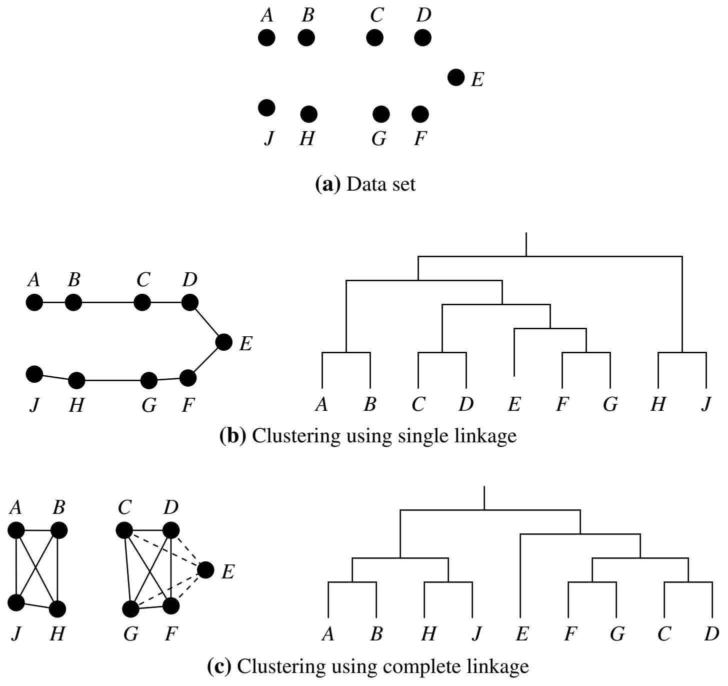
Example 10.4 **Single versus complete linkages.** Let us apply hierarchical clustering to the data set of Figure 10.8(a). Figure 10.8(b) shows the dendrogram using single linkage. Figure 10.8(c) shows the case using complete linkage, where the edges between clusters $\{A, B, J, H\}$ and $\{C, D, G, F, E\}$ are omitted for ease of presentation. This example shows that by using single linkages we can find hierarchical clusters defined by local proximity, whereas complete linkage tends to find clusters opting for global closeness. ■

There are variations of the four essential linkage measures just discussed. For example, we can measure the distance between two clusters by the distance between the centroids (i.e., the central objects) of the clusters.

10.3.3 BIRCH: Multiphase Hierarchical Clustering Using Clustering Feature Trees

Balanced Iterative Reducing and Clustering using Hierarchies (BIRCH) is designed for clustering a large amount of numeric data by integrating hierarchical clustering (at the initial *microclustering* stage) and other clustering methods such as iterative partitioning (at the later *macroclustering* stage). It overcomes the two difficulties in agglomerative clustering methods: (1) scalability and (2) the inability to undo what was done in the previous step.

BIRCH uses the notions of *clustering feature* to summarize a cluster, and *clustering feature tree* (*CF-tree*) to represent a cluster hierarchy. These structures help



A
B
C
D
E
J
H
G
F
(a) Data set
A B C D E F G H J
(b) Clustering using single linkage
A B H J E F G C D
(c) Clustering using complete linkage

Figure 10.8 Hierarchical clustering using single and complete linkages.

the clustering method achieve good speed and scalability in large or even streaming databases, and also make it effective for incremental and dynamic clustering of incoming objects.

Consider a cluster of n d-dimensional data objects or points. The **clustering feature** (**CF**) of the cluster is a 3-D vector summarizing information about clusters of objects. It is defined as

$$CF = \langle n, LS, SS \rangle, \tag{10.7}$$

where LS is the linear sum of the n points (i.e., $\sum_{i=1}^{n} \boldsymbol{x_i}$), and SS is the square sum of the data points (i.e., $\sum_{i=1}^{n} \boldsymbol{x_i}^2$).

A clustering feature is essentially a summary of the statistics for the given cluster. Using a clustering feature, we can easily derive many useful statistics of a cluster. For example, the cluster's centroid, $\boldsymbol{x_0}$, radius, R, and diameter, D, are

$$\boldsymbol{x_0} = \frac{\sum\limits_{i=1}^{n} \boldsymbol{x_i}}{n} = \frac{LS}{n}, \tag{10.8}$$

$$R = \sqrt{\frac{\sum_{i=1}^{n}(\boldsymbol{x_i} - \boldsymbol{x_0})^2}{n}} = \sqrt{\frac{nSS - 2LS^2 + nLS}{n^2}}, \tag{10.9}$$

$$D = \sqrt{\frac{\sum_{i=1}^{n}\sum_{j=1}^{n}(\boldsymbol{x_i} - \boldsymbol{x_j})^2}{n(n-1)}} = \sqrt{\frac{2nSS - 2LS^2}{n(n-1)}}. \tag{10.10}$$

Here, R is the average distance from member objects to the centroid, and D is the average pairwise distance within a cluster. Both R and D reflect the tightness of the cluster around the centroid.

Summarizing a cluster using the clustering feature can avoid storing the detailed information about individual objects or points. Instead, we only need a constant size of space to store the clustering feature. This is the key to BIRCH efficiency in space. Moreover, clustering features are *additive*. That is, for two disjoint clusters, C_1 and C_2, with the clustering features $CF_1 = \langle n_1, LS_1, SS_1\rangle$ and $CF_2 = \langle n_2, LS_2, SS_2\rangle$, respectively, the clustering feature for the cluster that formed by merging C_1 and C_2 is simply

$$CF_1 + CF_2 = \langle n_1 + n_2, LS_1 + LS_2, SS_1 + SS_2\rangle. \tag{10.11}$$

Example 10.5 Clustering feature. Suppose there are three points, $(2,5), (3,2)$, and $(4,3)$, in a cluster, C_1. The clustering feature of C_1 is

$$CF_1 = \langle 3, (2+3+4, 5+2+3), (2^2+3^2+4^2, 5^2+2^2+3^2)\rangle = \langle 3, (9,10), (29,38)\rangle.$$

Suppose that C_1 is disjoint to a second cluster, C_2, where $CF_2 = \langle 3, (35,36), (417,440)\rangle$. The clustering feature of a new cluster, C_3, that is formed by merging C_1 and C_2, is derived by adding CF_1 and CF_2. That is,

$$CF_3 = \langle 3+3, (9+35, 10+36), (29+417, 38+440)\rangle = \langle 6, (44,46), (446,478)\rangle. \quad \blacksquare$$

A **CF-tree** is a height-balanced tree that stores the clustering features for a hierarchical clustering. An example is shown in Figure 10.9. By definition, a nonleaf node in a tree has descendants or "children." The nonleaf nodes store sums of the CFs of their children, and thus summarize clustering information about their children. A CF-tree has two parameters: *branching factor*, B, and *threshold*, T. The branching factor specifies the maximum number of children per nonleaf node. The threshold parameter specifies the maximum diameter of subclusters stored at the leaf nodes of the tree. These two parameters implicitly control the resulting tree's size.

Given a limited amount of main memory, an important consideration in BIRCH is to minimize the time required for input/output (I/O). BIRCH applies a *multiphase* clustering technique: A single scan of the data set yields a basic, good clustering, and

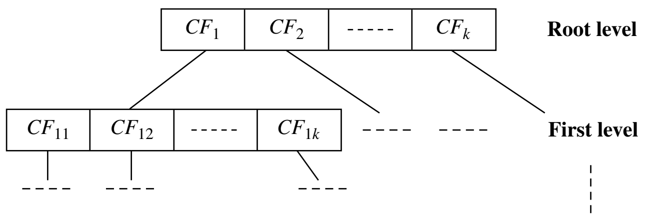


Figure 10.9 CF-tree structure.

one or more additional scans can optionally be used to further improve the quality. The primary phases are

- **Phase 1:** BIRCH scans the database to build an initial in-memory CF-tree, which can be viewed as a multilevel compression of the data that tries to preserve the data's inherent clustering structure.
- **Phase 2:** BIRCH applies a (selected) clustering algorithm to cluster the leaf nodes of the CF-tree, which removes sparse clusters as outliers and groups dense clusters into larger ones.

For Phase 1, the CF-tree is built dynamically as objects are inserted. Thus, the method is incremental. An object is inserted into the closest leaf entry (subcluster). If the diameter of the subcluster stored in the leaf node after insertion is larger than the threshold value, then the leaf node and possibly other nodes are split. After the insertion of the new object, information about the object is passed toward the root of the tree. The size of the CF-tree can be changed by modifying the threshold. If the size of the memory that is needed for storing the CF-tree is larger than the size of the main memory, then a larger threshold value can be specified and the CF-tree is rebuilt.

The rebuild process is performed by building a new tree from the leaf nodes of the old tree. Thus, the process of rebuilding the tree is done without the necessity of rereading all the objects or points. This is similar to the insertion and node split in the construction of B+-trees. Therefore, for building the tree, data has to be read just once. Some heuristics and methods have been introduced to deal with outliers and improve the quality of CF-trees by additional scans of the data. Once the CF-tree is built, any clustering algorithm, such as a typical partitioning algorithm, can be used with the CF-tree in Phase 2.

"How effective is BIRCH?" The time complexity of the algorithm is $O(n)$, where n is the number of objects to be clustered. Experiments have shown the linear scalability of the algorithm with respect to the number of objects, and good quality of clustering of the data. However, since each node in a CF-tree can hold only a limited number of entries due to its size, a CF-tree node does not always correspond to what a user may consider a natural cluster. Moreover, if the clusters are not spherical in shape, BIRCH does not perform well because it uses the notion of radius or diameter to control the boundary of a cluster.

The ideas of clustering features and CF-trees have been applied beyond BIRCH. The ideas have been borrowed by many others to tackle problems of clustering streaming and dynamic data.

10.3.4 Chameleon: Multiphase Hierarchical Clustering Using Dynamic Modeling

Chameleon is a hierarchical clustering algorithm that uses dynamic modeling to determine the similarity between pairs of clusters. In Chameleon, cluster similarity is assessed based on (1) how well connected objects are within a cluster and (2) the proximity of clusters. That is, two clusters are merged if their *interconnectivity* is high and they are *close together*. Thus, Chameleon does not depend on a static, user-supplied model and can automatically adapt to the internal characteristics of the clusters being merged. The merge process facilitates the discovery of natural and homogeneous clusters and applies to all data types as long as a similarity function can be specified.

Figure 10.10 illustrates how Chameleon works. Chameleon uses a k-nearest-neighbor graph approach to construct a sparse graph, where each vertex of the graph represents a data object, and there exists an edge between two vertices (objects) if one object is among the k-most similar objects to the other. The edges are weighted to reflect the similarity between objects. Chameleon uses a graph partitioning algorithm to partition the k-nearest-neighbor graph into a large number of relatively small subclusters such that it minimizes the **edge cut**. That is, a cluster C is partitioned into subclusters C_i and C_j so as to minimize the *weight of the edges* that would be cut should C be bisected into C_i and C_j. It assesses the *absolute* interconnectivity between clusters C_i and C_j.

Chameleon then uses an agglomerative hierarchical clustering algorithm that iteratively merges subclusters based on their similarity. To determine the pairs of most similar subclusters, it takes into account both the interconnectivity and the closeness of the clusters. Specifically, Chameleon determines the similarity between each pair of clusters C_i and C_j according to their *relative interconnectivity*, $RI(C_i, C_j)$, and their *relative closeness*, $RC(C_i, C_j)$.

- The **relative interconnectivity**, $RI(C_i, C_j)$, between two clusters, C_i and C_j, is defined as the absolute interconnectivity between C_i and C_j, normalized with respect to the

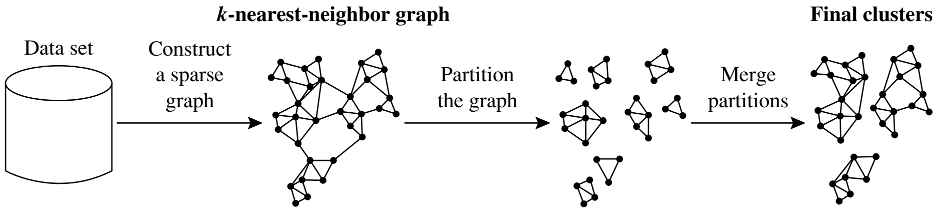


Figure 10.10 Chameleon: hierarchical clustering based on k-nearest neighbors and dynamic modeling. *Source:* Based on Karypis, Han, and Kumar [KHK99].

internal interconnectivity of the two clusters, C_i and C_j. That is,

$$RI(C_i, C_j) = \frac{|EC_{\{C_i,C_j\}}|}{\frac{1}{2}(|EC_{C_i}| + |EC_{C_j}|)}, \tag{10.12}$$

where $EC_{\{C_i,C_j\}}$ is the edge cut as previously defined for a cluster containing both C_i and C_j. Similarly, EC_{C_i} (or EC_{C_j}) is the minimum sum of the cut edges that partition C_i (or C_j) into two roughly equal parts.

- The **relative closeness**, $RC(C_i, C_j)$, between a pair of clusters, C_i and C_j, is the absolute closeness between C_i and C_j, normalized with respect to the internal closeness of the two clusters, C_i and C_j. It is defined as

$$RC(C_i, C_j) = \frac{\overline{S}_{EC_{\{C_i,C_j\}}}}{\frac{|C_i|}{|C_i|+|C_j|}\overline{S}_{EC_{C_i}} + \frac{|C_j|}{|C_i|+|C_j|}\overline{S}_{EC_{C_j}}}, \tag{10.13}$$

where $\overline{S}_{EC_{\{C_i,C_j\}}}$ is the average weight of the edges that connect vertices in C_i to vertices in C_j, and $\overline{S}_{EC_{C_i}}$ (or $\overline{S}_{EC_{C_j}}$) is the average weight of the edges that belong to the min-cut bisector of cluster C_i (or C_j).

Chameleon has been shown to have greater power at discovering arbitrarily shaped clusters of high quality than several well-known algorithms such as BIRCH and density-based DBSCAN (Section 10.4.1). However, the processing cost for high-dimensional data may require $O(n^2)$ time for n objects in the worst case.

10.3.5 Probabilistic Hierarchical Clustering

Algorithmic hierarchical clustering methods using linkage measures tend to be easy to understand and are often efficient in clustering. They are commonly used in many clustering analysis applications. However, algorithmic hierarchical clustering methods can suffer from several drawbacks. First, choosing a good distance measure for hierarchical clustering is often far from trivial. Second, to apply an algorithmic method, the data objects cannot have any missing attribute values. In the case of data that are partially observed (i.e., some attribute values of some objects are missing), it is not easy to apply an algorithmic hierarchical clustering method because the distance computation cannot be conducted. Third, most of the algorithmic hierarchical clustering methods are heuristic, and at each step locally search for a good merging/splitting decision. Consequently, the optimization goal of the resulting cluster hierarchy can be unclear.

Probabilistic hierarchical clustering aims to overcome some of these disadvantages by using probabilistic models to measure distances between clusters.

One way to look at the clustering problem is to regard the set of data objects to be clustered as a sample of the underlying data generation mechanism to be analyzed or, formally, the *generative model.* For example, when we conduct clustering analysis on a set of marketing surveys, we assume that the surveys collected are a sample of the opinions of all possible customers. Here, the data generation mechanism is a probability distribution of opinions with respect to different customers, which cannot be obtained directly and completely. The task of clustering is to estimate the generative model as accurately as possible using the observed data objects to be clustered.

In practice, we can assume that the data generative models adopt common distribution functions, such as Gaussian distribution or Bernoulli distribution, which are governed by parameters. The task of learning a generative model is then reduced to finding the parameter values for which the model best fits the observed data set.

Example 10.6 **Generative model.** Suppose we are given a set of 1-D points $X = \{x_1, \ldots, x_n\}$ for clustering analysis. Let us assume that the data points are generated by a Gaussian distribution,

$$\mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \tag{10.14}$$

where the parameters are μ (the mean) and σ^2 (the variance).

The probability that a point $x_i \in X$ is then generated by the model is

$$P(x_i|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}. \tag{10.15}$$

Consequently, the likelihood that X is generated by the model is

$$L(\mathcal{N}(\mu, \sigma^2) : X) = P(X|\mu, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}. \tag{10.16}$$

The task of learning the generative model is to find the parameters μ and σ^2 such that the likelihood $L(\mathcal{N}(\mu, \sigma^2) : X)$ is maximized, that is, finding

$$\mathcal{N}(\mu_0, \sigma_0^2) = \arg\max\{L(\mathcal{N}(\mu, \sigma^2) : X)\}, \tag{10.17}$$

where $\max\{L(\mathcal{N}(\mu, \sigma^2) : X)\}$ is called the *maximum likelihood.* ■

Given a set of objects, the quality of a cluster formed by all the objects can be measured by the maximum likelihood. For a set of objects partitioned into m clusters $C_1, \ldots, C_m$, the quality can be measured by

$$Q(\{C_1, \ldots, C_m\}) = \prod_{i=1}^{m} P(C_i), \tag{10.18}$$

where $P()$ is the maximum likelihood. If we merge two clusters, C_{j_1} and C_{j_2}, into a cluster, $C_{j_1} \cup C_{j_2}$, then, the change in quality of the overall clustering is

$$\begin{aligned} &Q((\{C_1,\ldots,C_m\} - \{C_{j_1}, C_{j_2}\}) \cup \{C_{j_1} \cup C_{j_2}\}) - Q(\{C_1,\ldots,C_m\}) \\ &= \frac{\prod_{i=1}^{m} P(C_i) \cdot P(C_{j_1} \cup C_{j_2})}{P(C_{j_1})P(C_{j_2})} - \prod_{i=1}^{m} P(C_i) \\ &= \prod_{i=1}^{m} P(C_i) \left(\frac{P(C_{j_1} \cup C_{j_2})}{P(C_{j_1})P(C_{j_2})} - 1 \right). \end{aligned} \tag{10.19}$$

When choosing to merge two clusters in hierarchical clustering, $\prod_{i=1}^{m} P(C_i)$ is constant for any pair of clusters. Therefore, given clusters C_1 and C_2, the distance between them can be measured by

$$dist(C_i, C_j) = -\log \frac{P(C_1 \cup C_2)}{P(C_1)P(C_2)}. \tag{10.20}$$

A probabilistic hierarchical clustering method can adopt the agglomerative clustering framework, but use probabilistic models (Eq. 10.20) to measure the distance between clusters.

Upon close observation of Eq. (10.19), we see that merging two clusters may not always lead to an improvement in clustering quality, that is, $\frac{P(C_{j_1} \cup C_{j_2})}{P(C_{j_1})P(C_{j_2})}$ may be less than 1. For example, assume that Gaussian distribution functions are used in the model of Figure 10.11. Although merging clusters C_1 and C_2 results in a cluster that better fits a Gaussian distribution, merging clusters C_3 and C_4 lowers the clustering quality because no Gaussian functions can fit the merged cluster well.

Based on this observation, a probabilistic hierarchical clustering scheme can start with one cluster per object, and merge two clusters, C_i and C_j, if the distance between them is negative. In each iteration, we try to find C_i and C_j so as to maximize $\log \frac{P(C_i \cup C_j)}{P(C_i)P(C_j)}$. The iteration continues as long as $\log \frac{P(C_i \cup C_j)}{P(C_i)P(C_j)} > 0$, that is, as long as there is an improvement in clustering quality. The pseudocode is given in Figure 10.12.

Probabilistic hierarchical clustering methods are easy to understand, and generally have the same efficiency as algorithmic agglomerative hierarchical clustering methods; in fact, they share the same framework. Probabilistic models are more interpretable, but sometimes less flexible than distance metrics. Probabilistic models can handle partially observed data. For example, given a multidimensional data set where some objects have missing values on some dimensions, we can learn a Gaussian model on each dimension independently using the observed values on the dimension. The resulting cluster hierarchy accomplishes the optimization goal of fitting data to the selected probabilistic models.

A drawback of using probabilistic hierarchical clustering is that it outputs only one hierarchy with respect to a chosen probabilistic model. It cannot handle the uncertainty of cluster hierarchies. Given a data set, there may exist multiple hierarchies that

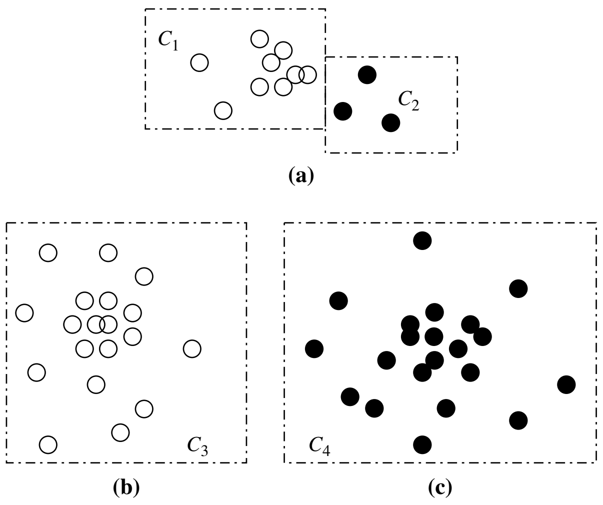


Figure 10.11 Merging clusters in probabilistic hierarchical clustering: (a) Merging clusters C_1 and C_2 leads to an increase in overall cluster quality, but merging clusters (b) C_3 and (c) C_4 does not.

Algorithm: A probabilistic hierarchical clustering algorithm.

Input:

- $D = \{\boldsymbol{o_1}, \ldots, \boldsymbol{o_n}\}$: a data set containing n objects;

Output: A hierarchy of clusters.

Method:

```
(1) create a cluster for each object $C_i = \{\boldsymbol{o_i}\}, 1 \le i \le n$;
(2) for $i = 1$ to $n$
(3)     find pair of clusters $C_i$ and $C_j$ such that $C_i, C_j = \arg\max_{i \neq j} \log \frac{P(C_i \cup C_j)}{P(C_i)P(C_j)}$;
(4)     if $\log \frac{P(C_i \cup C_j)}{P(C_i)P(C_j)} > 0$ then merge $C_i$ and $C_j$;
(5)     else stop;
```

Figure 10.12 A probabilistic hierarchical clustering algorithm.

fit the observed data. Neither algorithmic approaches nor probabilistic approaches can find the distribution of such hierarchies. Recently, Bayesian tree-structured models have been developed to handle such problems. Bayesian and other sophisticated probabilistic clustering methods are considered advanced topics and are not covered in this book.

10.4 Density-Based Methods

Partitioning and hierarchical methods are designed to find spherical-shaped clusters. They have difficulty finding clusters of arbitrary shape such as the "S" shape and oval clusters in Figure 10.13. Given such data, they would likely inaccurately identify convex regions, where noise or outliers are included in the clusters.

To find clusters of arbitrary shape, alternatively, we can model clusters as dense regions in the data space, separated by sparse regions. This is the main strategy behind *density-based clustering methods*, which can discover clusters of nonspherical shape. In this section, you will learn the basic techniques of density-based clustering by studying three representative methods, namely, DBSCAN (Section 10.4.1), OPTICS (Section 10.4.2), and DENCLUE (Section 10.4.3).

10.4.1 DBSCAN: Density-Based Clustering Based on Connected Regions with High Density

"How can we find dense regions in density-based clustering?" The *density* of an object $\boldsymbol{o}$ can be measured by the number of objects close to $\boldsymbol{o}$. **DBSCAN** (Density-Based Spatial Clustering of Applications with Noise) finds *core objects*, that is, objects that have dense neighborhoods. It connects core objects and their neighborhoods to form dense regions as clusters.

"How does **DBSCAN** *quantify the neighborhood of an object?"* A user-specified parameter $\epsilon > 0$ is used to specify the radius of a neighborhood we consider for every object. The **ϵ-neighborhood** of an object $\boldsymbol{o}$ is the space within a radius ϵ centered at $\boldsymbol{o}$.

Due to the fixed neighborhood size parameterized by ϵ, the **density of a neighborhood** can be measured simply by the number of objects in the neighborhood. To determine whether a neighborhood is dense or not, DBSCAN uses another user-specified

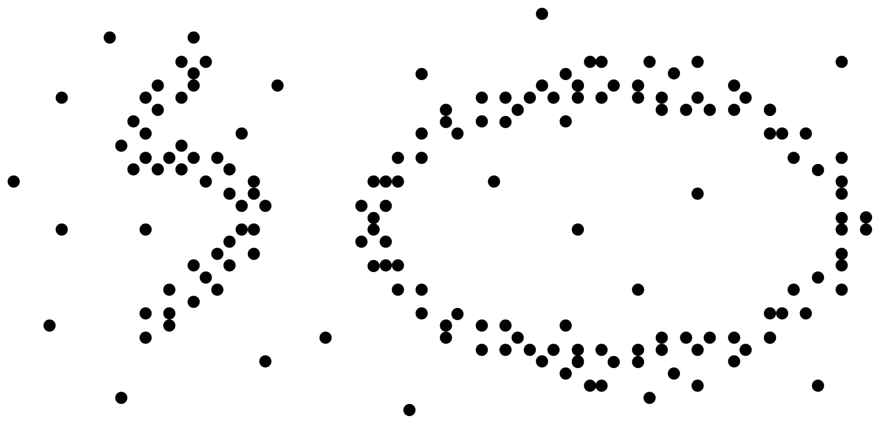


Figure 10.13 Clusters of arbitrary shape.

parameter, *MinPts*, which specifies the density threshold of dense regions. An object is a **core object** if the ϵ-neighborhood of the object contains at least *MinPts* objects. Core objects are the pillars of dense regions.

Given a set, D, of objects, we can identify all core objects with respect to the given parameters, ϵ and *MinPts*. The clustering task is therein reduced to using core objects and their neighborhoods to form dense regions, where the dense regions are clusters. For a core object $\boldsymbol{q}$ and an object $\boldsymbol{p}$, we say that $\boldsymbol{p}$ is **directly density-reachable** from $\boldsymbol{q}$ (with respect to ϵ and *MinPts*) if $\boldsymbol{p}$ is within the ϵ-neighborhood of $\boldsymbol{q}$. Clearly, an object $\boldsymbol{p}$ is directly density-reachable from another object $\boldsymbol{q}$ if and only if $\boldsymbol{q}$ is a core object and $\boldsymbol{p}$ is in the ϵ-neighborhood of $\boldsymbol{q}$. Using the directly density-reachable relation, a core object can "bring" all objects from its ϵ-neighborhood into a dense region.

"How can we assemble a large dense region using small dense regions centered by core objects?" In DBSCAN, $\boldsymbol{p}$ is **density-reachable** from $\boldsymbol{q}$ (with respect to ϵ and *MinPts* in D) if there is a chain of objects $\boldsymbol{p}_1, \ldots, \boldsymbol{p}_n$, such that $\boldsymbol{p}_1 = \boldsymbol{q}$, $\boldsymbol{p}_n = \boldsymbol{p}$, and $\boldsymbol{p}_{i+1}$ is directly density-reachable from $\boldsymbol{p}_i$ with respect to ϵ and *MinPts*, for $1 \leq i \leq n$, $\boldsymbol{p}_i \in D$. Note that density-reachability is not an equivalence relation because it is not symmetric. If both $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$ are core objects and $\boldsymbol{o}_1$ is density-reachable from $\boldsymbol{o}_2$, then $\boldsymbol{o}_2$ is density-reachable from $\boldsymbol{o}_1$. However, if $\boldsymbol{o}_2$ is a core object but $\boldsymbol{o}_1$ is not, then $\boldsymbol{o}_1$ may be density-reachable from $\boldsymbol{o}_2$, but not vice versa.

To connect core objects as well as their neighbors in a dense region, **DBSCAN** uses the notion of density-connectedness. Two objects $\boldsymbol{p}_1, \boldsymbol{p}_2 \in D$ are **density-connected** with respect to ϵ and *MinPts* if there is an object $\boldsymbol{q} \in D$ such that both $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ are density-reachable from $\boldsymbol{q}$ with respect to ϵ and *MinPts*. Unlike density-reachability, density-connectedness is an equivalence relation. It is easy to show that, for objects $\boldsymbol{o}_1$, $\boldsymbol{o}_2$, and $\boldsymbol{o}_3$, if $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$ are density-connected, and $\boldsymbol{o}_2$ and $\boldsymbol{o}_3$ are density-connected, then so are $\boldsymbol{o}_1$ and $\boldsymbol{o}_3$.

Example 10.7 Density-reachability and density-connectivity. Consider Figure 10.14 for a given ϵ represented by the radius of the circles, and, say, let $MinPts = 3$.

Of the labeled points, $\boldsymbol{m}, \boldsymbol{p}, \boldsymbol{o}, \boldsymbol{r}$ are core objects because each is in an ϵ-neighborhood containing at least three points. Object $\boldsymbol{q}$ is directly density-reachable from $\boldsymbol{m}$. Object $\boldsymbol{m}$ is directly density-reachable from $\boldsymbol{p}$ and vice versa.

Object $\boldsymbol{q}$ is (indirectly) density-reachable from $\boldsymbol{p}$ because $\boldsymbol{q}$ is directly density-reachable from $\boldsymbol{m}$ and $\boldsymbol{m}$ is directly density-reachable from $\boldsymbol{p}$. However, $\boldsymbol{p}$ is not density-reachable from $\boldsymbol{q}$ because $\boldsymbol{q}$ is not a core object. Similarly, $\boldsymbol{r}$ and $\boldsymbol{s}$ are density-reachable from $\boldsymbol{o}$ and $\boldsymbol{o}$ is density-reachable from $\boldsymbol{r}$. Thus, $\boldsymbol{o}$, $\boldsymbol{r}$, and $\boldsymbol{s}$ are all density-connected. ■

We can use the closure of density-connectedness to find connected dense regions as clusters. Each closed set is a **density-based cluster**. A subset $C \subseteq D$ is a cluster if (1) for any two objects $\boldsymbol{o}_1, \boldsymbol{o}_2 \in C$, $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$ are density-connected; and (2) there does not exist an object $\boldsymbol{o} \in C$ and another object $\boldsymbol{o}' \in (D - C)$ such that $\boldsymbol{o}$ and $\boldsymbol{o}'$ are density-connected.

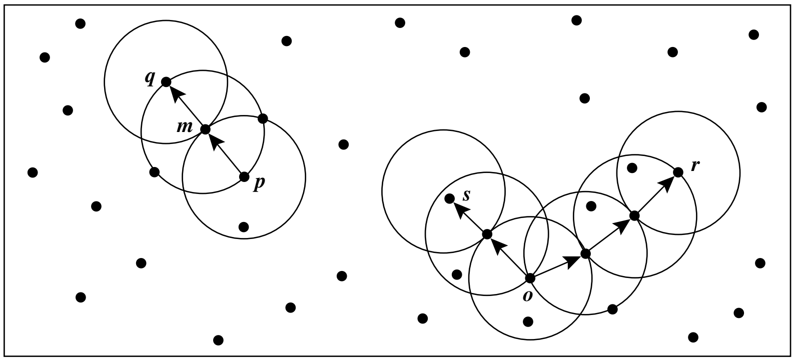


Figure 10.14 Density-reachability and density-connectivity in density-based clustering. *Source:* Based on Ester, Kriegel, Sander, and Xu [EKSX96].

"How does DBSCAN find clusters?" Initially, all objects in a given data set D are marked as "unvisited." DBSCAN randomly selects an unvisited object $\boldsymbol{p}$, marks $\boldsymbol{p}$ as "visited," and checks whether the ϵ-neighborhood of $\boldsymbol{p}$ contains at least *MinPts* objects. If not, $\boldsymbol{p}$ is marked as a noise point. Otherwise, a new cluster C is created for $\boldsymbol{p}$, and all the objects in the ϵ-neighborhood of $\boldsymbol{p}$ are added to a candidate set, N. DBSCAN iteratively adds to C those objects in N that do not belong to any cluster. In this process, for an object $\boldsymbol{p'}$ in N that carries the label "unvisited," DBSCAN marks it as "visited" and checks its ϵ-neighborhood. If the ϵ-neighborhood of $\boldsymbol{p'}$ has at least *MinPts* objects, those objects in the ϵ-neighborhood of $\boldsymbol{p'}$ are added to N. DBSCAN continues adding objects to C until C can no longer be expanded, that is, N is empty. At this time, cluster C is completed, and thus is output.

To find the next cluster, DBSCAN randomly selects an unvisited object from the remaining ones. The clustering process continues until all objects are visited. The pseudocode of the DBSCAN algorithm is given in Figure 10.15.

If a spatial index is used, the computational complexity of DBSCAN is $O(n \log n)$, where n is the number of database objects. Otherwise, the complexity is $O(n^2)$. With appropriate settings of the user-defined parameters, ϵ and *MinPts*, the algorithm is effective in finding arbitrary-shaped clusters.

10.4.2 OPTICS: Ordering Points to Identify the Clustering Structure

Although DBSCAN can cluster objects given input parameters such as ϵ (the maximum radius of a neighborhood) and *MinPts* (the minimum number of points required in the neighborhood of a core object), it encumbers users with the responsibility of selecting parameter values that will lead to the discovery of acceptable clusters. This is a problem associated with many other clustering algorithms. Such parameter settings

Algorithm: DBSCAN: a density-based clustering algorithm.

Input:

- D: a data set containing n objects,
- ϵ: the radius parameter, and
- *MinPts*: the neighborhood density threshold.

Output: A set of density-based clusters.

Method:

```
(1)  mark all objects as unvisited;
(2)  do
(3)      randomly select an unvisited object p;
(4)      mark p as visited;
(5)      if the ε-neighborhood of p has at least MinPts objects
(6)          create a new cluster C, and add p to C;
(7)          let N be the set of objects in the ε-neighborhood of p;
(8)          for each point p' in N
(9)              if p' is unvisited
(10)                 mark p' as visited;
(11)                 if the ε-neighborhood of p' has at least MinPts points,
                     add those points to N;
(12)             if p' is not yet a member of any cluster, add p' to C;
(13)         end for
(14)         output C;
(15)     else mark p as noise;
(16) until no object is unvisited;
```

Figure 10.15 DBSCAN algorithm.

are usually empirically set and difficult to determine, especially for real-world, high-dimensional data sets. Most algorithms are sensitive to these parameter values: Slightly different settings may lead to very different clusterings of the data. Moreover, real-world, high-dimensional data sets often have very skewed distributions such that their intrinsic clustering structure may not be well characterized by a single set of *global* density parameters.

Note that density-based clusters are monotonic with respect to the neighborhood threshold. That is, in DBSCAN, for a fixed *MinPts* value and two neighborhood thresholds, $\epsilon_1 < \epsilon_2$, a cluster C with respect to ϵ_1 and *MinPts* must be a subset of a cluster C' with respect to ϵ_2 and *MinPts*. This means that if two objects are in a density-based cluster, they must also be in a cluster with a lower density requirement.

To overcome the difficulty in using one set of global parameters in clustering analysis, a cluster analysis method called **OPTICS** was proposed. OPTICS does not explicitly produce a data set clustering. Instead, it outputs a **cluster ordering**. This is a linear list of all objects under analysis and represents the *density-based clustering structure* of the data. Objects in a denser cluster are listed closer to each other in the cluster ordering. This ordering is equivalent to density-based clustering obtained from a wide range of parameter settings. Thus, OPTICS does not require the user to provide a specific density threshold. The cluster ordering can be used to extract basic clustering information (e.g., cluster centers, or arbitrary-shaped clusters), derive the intrinsic clustering structure, as well as provide a visualization of the clustering.

To construct the different clusterings simultaneously, the objects are processed in a specific order. This order selects an object that is density-reachable with respect to the lowest ϵ value so that clusters with higher density (lower ϵ) will be finished first. Based on this idea, OPTICS needs two important pieces of information per object:

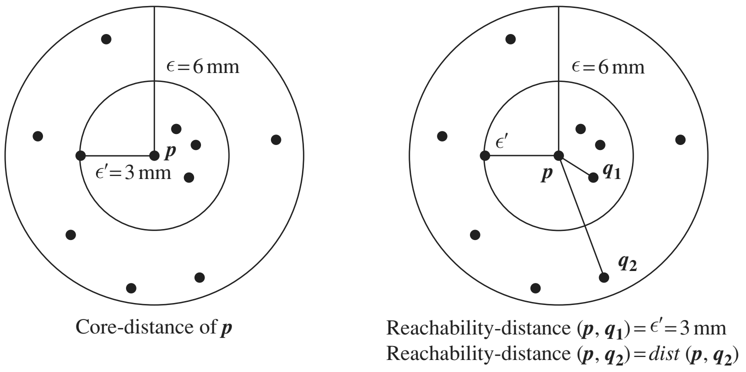
- The **core-distance** of an object $\boldsymbol{p}$ is the smallest value ϵ' such that the ϵ'-neighborhood of $\boldsymbol{p}$ has at least *MinPts* objects. That is, ϵ' is the minimum distance threshold that makes $\boldsymbol{p}$ a core object. If $\boldsymbol{p}$ is not a core object with respect to ϵ and *MinPts*, the core-distance of $\boldsymbol{p}$ is undefined.
- The **reachability-distance** to object $\boldsymbol{p}$ from $\boldsymbol{q}$ is the minimum radius value that makes $\boldsymbol{p}$ density-reachable from $\boldsymbol{q}$. According to the definition of density-reachability, $\boldsymbol{q}$ has to be a core object and $\boldsymbol{p}$ must be in the neighborhood of $\boldsymbol{q}$. Therefore, the reachability-distance from $\boldsymbol{q}$ to $\boldsymbol{p}$ is $\max\{\textit{core-distance}(\boldsymbol{q}), \textit{dist}(\boldsymbol{p}, \boldsymbol{q})\}$. If $\boldsymbol{q}$ is not a core object with respect to ϵ and *MinPts*, the reachability-distance to $\boldsymbol{p}$ from $\boldsymbol{q}$ is undefined.

  An object $\boldsymbol{p}$ may be directly reachable from multiple core objects. Therefore, $\boldsymbol{p}$ may have multiple reachability-distances with respect to different core objects. The smallest reachability-distance of $\boldsymbol{p}$ is of particular interest because it gives the shortest path for which $\boldsymbol{p}$ is connected to a dense cluster.

Example 10.8 **Core-distance and reachability-distance.** Figure 10.16 illustrates the concepts of core-distance and reachability-distance. Suppose that $\epsilon = 6$ mm and $MinPts = 5$. The core-distance of $\boldsymbol{p}$ is the distance, ϵ', between $\boldsymbol{p}$ and the fourth closest data object from $\boldsymbol{p}$. The reachability-distance of $\boldsymbol{q_1}$ from $\boldsymbol{p}$ is the core-distance of $\boldsymbol{p}$ (i.e., $\epsilon' = 3$ mm) because this is greater than the Euclidean distance from $\boldsymbol{p}$ to $\boldsymbol{q_1}$. The reachability-distance of $\boldsymbol{q_2}$ with respect to $\boldsymbol{p}$ is the Euclidean distance from $\boldsymbol{p}$ to $\boldsymbol{q_2}$ because this is greater than the core-distance of $\boldsymbol{p}$. ■

OPTICS computes an ordering of all objects in a given database and, for each object in the database, stores the core-distance and a suitable reachability-distance. OPTICS maintains a list called OrderSeeds to generate the output ordering. Objects in OrderSeeds are sorted by the reachability-distance from their respective closest core objects, that is, by the smallest reachability-distance of each object.

OPTICS begins with an arbitrary object from the input database as the current object, $\boldsymbol{p}$. It retrieves the ϵ-neighborhood of $\boldsymbol{p}$, determines the core-distance, and sets the reachability-distance to *undefined.* The current object, $\boldsymbol{p}$, is then written to output.



$\epsilon = 6$ mm
p
$\epsilon' = 3$ mm
Core-distance of p
$\epsilon = 6$ mm
ϵ'
p
q_1
q_2
Reachability-distance $(p, q_1) = \epsilon' = 3$ mm
Reachability-distance $(p, q_2) = dist\ (p, q_2)$

Figure 10.16 OPTICS terminology. *Source:* Based on Ankerst, Breunig, Kriegel, and Sander [ABKS99].

If $\boldsymbol{p}$ is not a core object, OPTICS simply moves on to the next object in the OrderSeeds list (or the input database if OrderSeeds is empty). If $\boldsymbol{p}$ is a core object, then for each object, $\boldsymbol{q}$, in the ϵ-neighborhood of $\boldsymbol{p}$, OPTICS updates its reachability-distance from $\boldsymbol{p}$ and inserts $\boldsymbol{q}$ into OrderSeeds if $\boldsymbol{q}$ has not yet been processed. The iteration continues until the input is fully consumed and OrderSeeds is empty.

A data set's cluster ordering can be represented graphically, which helps to visualize and understand the clustering structure in a data set. For example, Figure 10.17 is the reachability plot for a simple 2-D data set, which presents a general overview of how the data are structured and clustered. The data objects are plotted in the clustering order (horizontal axis) together with their respective reachability-distances (vertical axis). The three Gaussian "bumps" in the plot reflect three clusters in the data set. Methods have also been developed for viewing clustering structures of high-dimensional data at various levels of detail.

The structure of the OPTICS algorithm is very similar to that of DBSCAN. Consequently, the two algorithms have the same time complexity. The complexity is $O(n \log n)$ if a spatial index is used, and $O(n^2)$ otherwise, where n is the number of objects.

10.4.3 DENCLUE: Clustering Based on Density Distribution Functions

Density estimation is a core issue in density-based clustering methods. **DENCLUE** (DENsity-based CLUstEring) is a clustering method based on a set of density distribution functions. We first give some background on density estimation, and then describe the DENCLUE algorithm.

In probability and statistics, **density estimation** is the estimation of an unobservable underlying probability density function based on a set of observed data. In the context of density-based clustering, the unobservable underlying probability density function is the true distribution of the population of all possible objects to be analyzed. The observed data set is regarded as a random sample from that population.

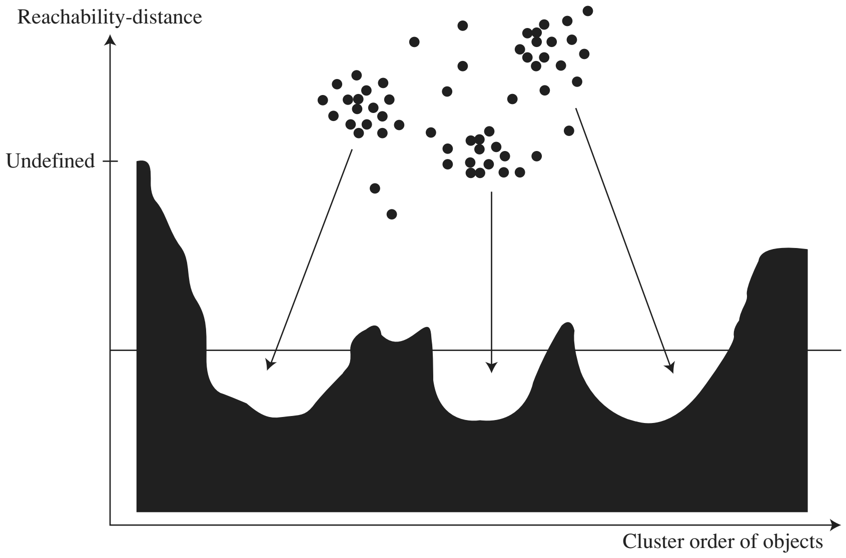


Figure 10.17 Cluster ordering in OPTICS. *Source:* Adapted from Ankerst, Breunig, Kriegel, and Sander [ABKS99].

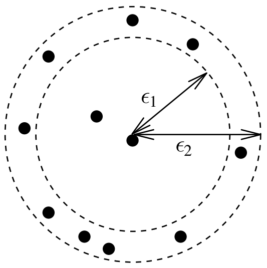


Figure 10.18 The subtlety in density estimation in DBSCAN and OPTICS: Increasing the neighborhood radius slightly from ϵ_1 to ϵ_2 results in a much higher density.

In DBSCAN and OPTICS, density is calculated by counting the number of objects in a neighborhood defined by a radius parameter, ϵ. Such density estimates can be highly sensitive to the radius value used. For example, in Figure 10.18, the density changes significantly as the radius increases by a small amount.

To overcome this problem, **kernel density estimation** can be used, which is a nonparametric density estimation approach from statistics. The general idea behind kernel density estimation is simple. We treat an observed object as an indicator of high-probability density in the surrounding region. The probability density at a point depends on the distances from this point to the observed objects.

Formally, let $\boldsymbol{x_1}, \ldots, \boldsymbol{x_n}$ be an independent and identically distributed sample of a random variable f. The *kernel density approximation of the probability density function* is

$$\hat{f}_h(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{\boldsymbol{x} - \boldsymbol{x_i}}{h}\right), \tag{10.21}$$

where $K()$ is a kernel and h is the bandwidth serving as a smoothing parameter. A **kernel** can be regarded as a function modeling the influence of a sample point within its neighborhood. Technically, a kernel $K()$ is a non-negative real-valued integrable function that should satisfy two requirements: $\int_{-\infty}^{+\infty} K(u)du = 1$ and $K(-u) = K(u)$ for all values of u. A frequently used kernel is a standard Gaussian function with a mean of 0 and a variance of 1:

$$K\left(\frac{\boldsymbol{x} - \boldsymbol{x_i}}{h}\right) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(\boldsymbol{x} - \boldsymbol{x_i})^2}{2h^2}}. \tag{10.22}$$

DENCLUE uses a Gaussian kernel to estimate density based on the given set of objects to be clustered. A point $\boldsymbol{x^*}$ is called a **density attractor** if it is a local maximum of the estimated density function. To avoid trivial local maximum points, DENCLUE uses a noise threshold, ξ, and only considers those density attractors $\boldsymbol{x^*}$ such that $\hat{f}(\boldsymbol{x^*}) \geq \xi$. These nontrivial density attractors are the centers of clusters.

Objects under analysis are assigned to clusters through density attractors using a stepwise hill-climbing procedure. For an object, $\boldsymbol{x}$, the hill-climbing procedure starts from $\boldsymbol{x}$ and is guided by the gradient of the estimated density function. That is, the density attractor for $\boldsymbol{x}$ is computed as

$$\begin{aligned} \boldsymbol{x^0} &= \boldsymbol{x} \\ \boldsymbol{x^{j+1}} &= \boldsymbol{x^j} + \delta \frac{\nabla \hat{f}(\boldsymbol{x^j})}{|\nabla \hat{f}(\boldsymbol{x^j})|}, \end{aligned} \tag{10.23}$$

where δ is a parameter to control the speed of convergence, and

$$\nabla \hat{f}(\boldsymbol{x}) = \frac{1}{h^{d+2} n \sum_{i=1}^{n} K\left(\frac{\boldsymbol{x} - \boldsymbol{x_i}}{h}\right)(\boldsymbol{x_i} - \boldsymbol{x})}. \tag{10.24}$$

The hill-climbing procedure stops at step $k > 0$ if $\hat{f}(\boldsymbol{x^{k+1}}) < \hat{f}(\boldsymbol{x^k})$, and assigns $\boldsymbol{x}$ to the density attractor $\boldsymbol{x^*} = \boldsymbol{x^k}$. An object $\boldsymbol{x}$ is an outlier or noise if it converges in the hill-climbing procedure to a local maximum $\boldsymbol{x^*}$ with $\hat{f}(\boldsymbol{x^*}) < \xi$.

A cluster in DENCLUE is a set of density attractors X and a set of input objects C such that each object in C is assigned to a density attractor in X, and there exists a path between every pair of density attractors where the density is above ξ. By using multiple density attractors connected by paths, DENCLUE can find clusters of arbitrary shape.

DENCLUE has several advantages. It can be regarded as a generalization of several well-known clustering methods such as single-linkage approaches and DBSCAN. Moreover, DENCLUE is invariant against noise. The kernel density estimation can effectively reduce the influence of noise by uniformly distributing noise into the input data.

10.5 Grid-Based Methods

The clustering methods discussed so far are data-driven—they partition the set of objects and adapt to the distribution of the objects in the embedding space. Alternatively, a **grid-based clustering** method takes a space-driven approach by partitioning the embedding space into *cells* independent of the distribution of the input objects.

The *grid-based clustering* approach uses a multiresolution grid data structure. It quantizes the object space into a finite number of cells that form a grid structure on which all of the operations for clustering are performed. The main advantage of the approach is its fast processing time, which is typically independent of the number of data objects, yet dependent on only the number of cells in each dimension in the quantized space.

In this section, we illustrate grid-based clustering using two typical examples. STING (Section 10.5.1) explores statistical information stored in the grid cells. CLIQUE (Section 10.5.2) represents a grid- and density-based approach for subspace clustering in a high-dimensional data space.

10.5.1 STING: STatistical INformation Grid

STING is a grid-based multiresolution clustering technique in which the embedding spatial area of the input objects is divided into rectangular cells. The space can be divided in a hierarchical and recursive way. Several levels of such rectangular cells correspond to different levels of resolution and form a hierarchical structure: Each cell at a high level is partitioned to form a number of cells at the next lower level. Statistical information regarding the attributes in each grid cell, such as the mean, maximum, and minimum values, is precomputed and stored as *statistical parameters.* These statistical parameters are useful for query processing and for other data analysis tasks.

Figure 10.19 shows a hierarchical structure for STING clustering. The statistical parameters of higher-level cells can easily be computed from the parameters of the lower-level cells. These parameters include the following: the attribute-independent parameter, *count*; and the attribute-dependent parameters, *mean*, *stdev* (standard deviation), *min* (minimum), *max* (maximum), and the type of *distribution* that the attribute value in the cell follows such as *normal, uniform*, *exponential*, or *none* (if the distribution is unknown). Here, the attribute is a selected measure for analysis such as *price* for house objects. When the data are loaded into the database, the parameters *count*, *mean*, *stdev*, *min*, and *max* of the bottom-level cells are calculated directly from the data. The value of *distribution* may either be assigned by the user if the distribution type is known

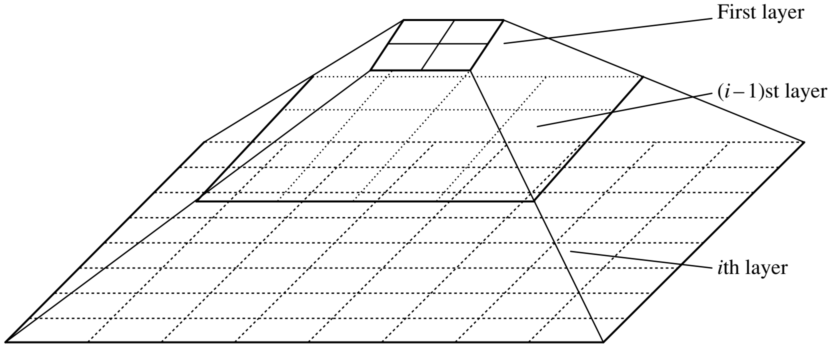


Figure 10.19 Hierarchical structure for STING clustering.

beforehand or obtained by hypothesis tests such as the χ^2 test. The type of distribution of a higher-level cell can be computed based on the majority of distribution types of its corresponding lower-level cells in conjunction with a threshold filtering process. If the distributions of the lower-level cells disagree with each other and fail the threshold test, the distribution type of the high-level cell is set to *none*.

"How is this statistical information useful for query answering?" The statistical parameters can be used in a top-down, grid-based manner as follows. First, a layer within the hierarchical structure is determined from which the query-answering process is to start. This layer typically contains a small number of cells. For each cell in the current layer, we compute the confidence interval (or estimated probability range) reflecting the cell's relevancy to the given query. The irrelevant cells are removed from further consideration. Processing of the next lower level examines only the remaining relevant cells. This process is repeated until the bottom layer is reached. At this time, if the query specification is met, the regions of relevant cells that satisfy the query are returned. Otherwise, the data that fall into the relevant cells are retrieved and further processed until they meet the query's requirements.

An interesting property of STING is that it approaches the clustering result of DBSCAN if the granularity approaches 0 (i.e., toward very low-level data). In other words, using the count and cell size information, dense clusters can be identified approximately using STING. Therefore, STING can also be regarded as a density-based clustering method.

"What advantages does STING offer over other clustering methods?" STING offers several advantages: (1) the grid-based computation is *query-independent* because the statistical information stored in each cell represents the summary information of the data in the grid cell, independent of the query; (2) the grid structure facilitates parallel processing and incremental updating; and (3) the method's efficiency is a major advantage: STING goes through the database once to compute the statistical parameters of the cells, and hence the time complexity of generating clusters is $O(n)$, where n is the total number of objects. After generating the hierarchical structure, the query processing time

is $O(g)$, where g is the total number of grid cells at the lowest level, which is usually much smaller than n.

Because STING uses a multiresolution approach to cluster analysis, the quality of STING clustering depends on the granularity of the lowest level of the grid structure. If the granularity is very fine, the cost of processing will increase substantially; however, if the bottom level of the grid structure is too coarse, it may reduce the quality of cluster analysis. Moreover, STING does not consider the spatial relationship between the children and their neighboring cells for construction of a parent cell. As a result, the shapes of the resulting clusters are isothetic, that is, all the cluster boundaries are either horizontal or vertical, and no diagonal boundary is detected. This may lower the quality and accuracy of the clusters despite the fast processing time of the technique.

10.5.2 CLIQUE: An Apriori-like Subspace Clustering Method

A data object often has tens of attributes, many of which may be irrelevant. The values of attributes may vary considerably. These factors can make it difficult to locate clusters that span the entire data space. It may be more meaningful to instead search for clusters within different *subspaces* of the data. For example, consider a health-informatics application where patient records contain extensive attributes describing personal information, numerous symptoms, conditions, and family history.

Finding a nontrivial group of patients for which all or even most of the attributes strongly agree is unlikely. In bird flu patients, for instance, the *age*, *gender*, and *job* attributes may vary dramatically within a wide range of values. Thus, it can be difficult to find such a cluster within the entire data space. Instead, by searching in subspaces, we may find a cluster of similar patients in a lower-dimensional space (e.g., patients who are similar to one other with respect to symptoms like high fever, cough but no runny nose, and aged between 3 and 16).

CLIQUE (CLustering In QUEst) is a simple grid-based method for finding density-based clusters in subspaces. CLIQUE partitions each dimension into nonoverlapping intervals, thereby partitioning the entire embedding space of the data objects into cells. It uses a density threshold to identify *dense* cells and *sparse* ones. A cell is dense if the number of objects mapped to it exceeds the density threshold.

The main strategy behind CLIQUE for identifying a candidate search space uses the monotonicity of dense cells with respect to dimensionality. This is based on the *Apriori property* used in frequent pattern and association rule mining (Chapter 6). In the context of clusters in subspaces, the monotonicity says the following. A k-dimensional cell c $(k > 1)$ can have at least l points only if every $(k-1)$-dimensional projection of c, which is a cell in a $(k-1)$-dimensional subspace, has at least l points. Consider Figure 10.20, where the embedding data space contains three dimensions: *age, salary*, and *vacation*. A 2-D cell, say in the subspace formed by *age* and *salary*, contains l points only if the projection of this cell in every dimension, that is, *age* and *salary*, respectively, contains at least l points.

CLIQUE performs clustering in two steps. In the first step, CLIQUE partitions the d-dimensional data space into nonoverlapping rectangular units, identifying the dense units among these. CLIQUE finds dense cells in all of the subspaces. To do so,

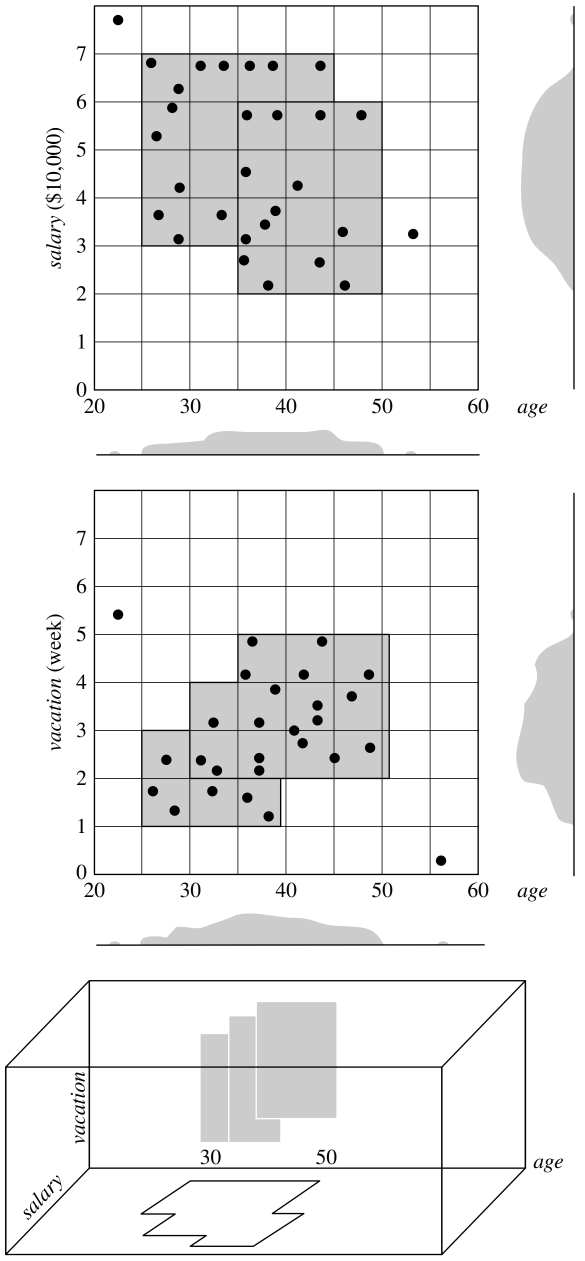


Figure 10.20 Dense units found with respect to *age* for the dimensions *salary* and *vacation* are intersected to provide a candidate search space for dense units of higher dimensionality.

CLIQUE partitions every dimension into intervals, and identifies intervals containing at least l points, where l is the density threshold. CLIQUE then iteratively joins two k-dimensional dense cells, c_1 and c_2, in subspaces $(D_{i_1},\ldots,D_{i_k})$ and $(D_{j_1},\ldots,D_{j_k})$, respectively, if $D_{i_1}=D_{j_1},\ldots,D_{i_{k-1}}=D_{j_{k-1}}$, and c_1 and c_2 share the same intervals in those dimensions. The join operation generates a new $(k+1)$-dimensional candidate cell c in space $(D_{i_1},\ldots,D_{i_{k-1}},D_{i_k},D_{j_k})$. CLIQUE checks whether the number of points in c passes the density threshold. The iteration terminates when no candidates can be generated or no candidate cells are dense.

In the second step, CLIQUE uses the dense cells in each subspace to assemble clusters, which can be of arbitrary shape. The idea is to apply the Minimum Description Length (MDL) principle (Chapter 8) to use the *maximal regions* to cover connected dense cells, where a maximal region is a hyperrectangle where every cell falling into this region is dense, and the region cannot be extended further in any dimension in the subspace. Finding the best description of a cluster in general is NP-Hard. Thus, CLIQUE adopts a simple greedy approach. It starts with an arbitrary dense cell, finds a maximal region covering the cell, and then works on the remaining dense cells that have not yet been covered. The greedy method terminates when all dense cells are covered.

"How effective is CLIQUE?" CLIQUE automatically finds subspaces of the highest dimensionality such that high-density clusters exist in those subspaces. It is insensitive to the order of input objects and does not presume any canonical data distribution. It scales linearly with the size of the input and has good scalability as the number of dimensions in the data is increased. However, obtaining a meaningful clustering is dependent on proper tuning of the grid size (which is a stable structure here) and the density threshold. This can be difficult in practice because the grid size and density threshold are used across all combinations of dimensions in the data set. Thus, the accuracy of the clustering results may be degraded at the expense of the method's simplicity. Moreover, for a given dense region, all projections of the region onto lower-dimensionality subspaces will also be dense. This can result in a large overlap among the reported dense regions. Furthermore, it is difficult to find clusters of rather different densities within different dimensional subspaces.

Several extensions to this approach follow a similar philosophy. For example, we can think of a grid as a set of fixed bins. Instead of using fixed bins for each of the dimensions, we can use an adaptive, data-driven strategy to dynamically determine the bins for each dimension based on data distribution statistics. Alternatively, instead of using a density threshold, we may use entropy (Chapter 8) as a measure of the quality of subspace clusters.

10.6 Evaluation of Clustering

By now you have learned what clustering is and know several popular clustering methods. You may ask, "*When I try out a clustering method on a data set, how can I evaluate whether the clustering results are good?*" In general, *cluster evaluation* assesses the feasibility of clustering analysis on a data set and the quality of the results generated by a clustering method. The major tasks of clustering evaluation include the following:

- *Assessing clustering tendency.* In this task, for a given data set, we assess whether a nonrandom structure exists in the data. Blindly applying a clustering method on a data set will return clusters; however, the clusters mined may be misleading. Clustering analysis on a data set is meaningful only when there is a nonrandom structure in the data.
- *Determining the number of clusters in a data set.* A few algorithms, such as k-means, require the number of clusters in a data set as the parameter. Moreover, the number of clusters can be regarded as an interesting and important summary statistic of a data set. Therefore, it is desirable to estimate this number even before a clustering algorithm is used to derive detailed clusters.
- *Measuring clustering quality.* After applying a clustering method on a data set, we want to assess how good the resulting clusters are. A number of measures can be used. Some methods measure how well the clusters fit the data set, while others measure how well the clusters match the ground truth, if such truth is available. There are also measures that score clusterings and thus can compare two sets of clustering results on the same data set.

In the rest of this section, we discuss each of these three topics.

10.6.1 Assessing Clustering Tendency

Clustering tendency assessment determines whether a given data set has a non-random structure, which may lead to meaningful clusters. Consider a data set that does not have any non-random structure, such as a set of uniformly distributed points in a data space. Even though a clustering algorithm may return clusters for the data, those clusters are random and are not meaningful.

Example 10.9 **Clustering requires nonuniform distribution of data.** Figure 10.21 shows a data set that is uniformly distributed in 2-D data space. Although a clustering algorithm may still artificially partition the points into groups, the groups will unlikely mean anything significant to the application due to the uniform distribution of the data. ■

"How can we assess the clustering tendency of a data set?" Intuitively, we can try to measure the probability that the data set is generated by a uniform data distribution. This can be achieved using statistical tests for spatial randomness. To illustrate this idea, let's look at a simple yet effective statistic called the Hopkins Statistic.

The **Hopkins Statistic** is a spatial statistic that tests the spatial randomness of a variable as distributed in a space. Given a data set, D, which is regarded as a sample of

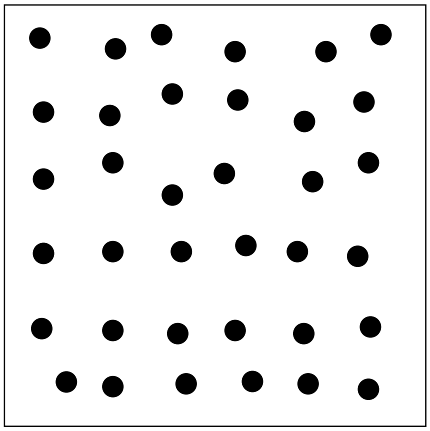


Figure 10.21 A data set that is uniformly distributed in the data space.

a random variable, o, we want to determine how far away o is from being uniformly distributed in the data space. We calculate the Hopkins Statistic as follows:

1. Sample n points, $\boldsymbol{p_1}, \ldots, \boldsymbol{p_n}$, uniformly from D. That is, each point in D has the same probability of being included in this sample. For each point, $\boldsymbol{p_i}$, we find the nearest neighbor of $\boldsymbol{p_i}$ $(1 \le i \le n)$ in D, and let x_i be the distance between $\boldsymbol{p_i}$ and its nearest neighbor in D. That is,

$$x_i = \min_{\boldsymbol{v} \in D}\{dist(\boldsymbol{p_i}, \boldsymbol{v})\}. \tag{10.25}$$

2. Sample n points, $\boldsymbol{q_1}, \ldots, \boldsymbol{q_n}$, uniformly from D. For each $\boldsymbol{q_i}$ $(1 \le i \le n)$, we find the nearest neighbor of $\boldsymbol{q_i}$ in $D - \{\boldsymbol{q_i}\}$, and let y_i be the distance between $\boldsymbol{q_i}$ and its nearest neighbor in $D - \{\boldsymbol{q_i}\}$. That is,

$$y_i = \min_{\boldsymbol{v} \in D, \boldsymbol{v} \neq \boldsymbol{q_i}}\{dist(\boldsymbol{q_i}, \boldsymbol{v})\}. \tag{10.26}$$

3. Calculate the Hopkins Statistic, H, as

$$H = \frac{\sum_{i=1}^{n} y_i}{\sum_{i=1}^{n} x_i + \sum_{i=1}^{n} y_i}. \tag{10.27}$$

"What does the Hopkins Statistic tell us about how likely data set D *follows a uniform distribution in the data space?"* If D were uniformly distributed, then $\sum_{i=1}^{n} y_i$ and $\sum_{i=1}^{n} x_i$ would be close to each other, and thus H would be about 0.5. However, if D were highly skewed, then $\sum_{i=1}^{n} y_i$ would be substantially smaller than $\sum_{i=1}^{n} x_i$ in expectation, and thus H would be close to 0.

Our null hypothesis is the *homogeneous hypothesis*—that D is uniformly distributed and thus contains no meaningful clusters. The *nonhomogeneous hypothesis* (i.e., that D is not uniformly distributed and thus contains clusters) is the alternative hypothesis. We can conduct the Hopkins Statistic test iteratively, using 0.5 as the threshold to reject the alternative hypothesis. That is, if $H > 0.5$, then it is unlikely that D has statistically significant clusters.

10.6.2 Determining the Number of Clusters

Determining the "right" number of clusters in a data set is important, not only because some clustering algorithms like k-means require such a parameter, but also because the appropriate number of clusters controls the proper granularity of cluster analysis. It can be regarded as finding a good balance between *compressibility* and *accuracy* in cluster analysis. Consider two extreme cases. What if you were to treat the entire data set as a cluster? This would maximize the compression of the data, but such a cluster analysis has no value. On the other hand, treating each object in a data set as a cluster gives the finest clustering resolution (i.e., most accurate due to the zero distance between an object and the corresponding cluster center). In some methods like k-means, this even achieves the best cost. However, having one object per cluster does not enable any data summarization.

Determining the number of clusters is far from easy, often because the "right" number is ambiguous. Figuring out what the right number of clusters should be often depends on the distribution's shape and scale in the data set, as well as the clustering resolution required by the user. There are many possible ways to estimate the number of clusters. Here, we briefly introduce a few simple yet popular and effective methods.

A simple method is to set the number of clusters to about $\sqrt{\frac{n}{2}}$ for a data set of n points. In expectation, each cluster has $\sqrt{2n}$ points.

The **elbow method** is based on the observation that increasing the number of clusters can help to reduce the sum of within-cluster variance of each cluster. This is because having more clusters allows one to capture finer groups of data objects that are more similar to each other. However, the marginal effect of reducing the sum of within-cluster variances may drop if too many clusters are formed, because splitting a cohesive cluster into two gives only a small reduction. Consequently, a heuristic for selecting the right number of clusters is to use the turning point in the curve of the sum of within-cluster variances with respect to the number of clusters.

Technically, given a number, $k > 0$, we can form k clusters on the data set in question using a clustering algorithm like k-means, and calculate the sum of within-cluster variances, $var(k)$. We can then plot the curve of var with respect to k. The first (or most significant) turning point of the curve suggests the "right" number.

More advanced methods can determine the number of clusters using information criteria or information theoretic approaches. Please refer to the bibliographic notes for further information (Section 10.9).

The "right" number of clusters in a data set can also be determined by **cross-validation**, a technique often used in classification (Chapter 8). First, divide the given data set, D, into m parts. Next, use $m-1$ parts to build a clustering model, and use the remaining part to test the quality of the clustering. For example, for each point in the test set, we can find the closest centroid. Consequently, we can use the sum of the squared distances between all points in the test set and the closest centroids to measure how well the clustering model fits the test set. For any integer $k > 0$, we repeat this process m times to derive clusterings of k clusters by using each part in turn as the test set. The average of the quality measure is taken as the overall quality measure. We can then compare the overall quality measure with respect to different values of k, and find the number of clusters that best fits the data.

10.6.3 Measuring Clustering Quality

Suppose you have assessed the clustering tendency of a given data set. You may have also tried to predetermine the number of clusters in the set. You can now apply one or multiple clustering methods to obtain clusterings of the data set. "*How good is the clustering generated by a method, and how can we compare the clusterings generated by different methods?*"

We have a few methods to choose from for measuring the quality of a clustering. In general, these methods can be categorized into two groups according to whether ground truth is available. Here, *ground truth* is the ideal clustering that is often built using human experts.

If ground truth is available, it can be used by **extrinsic methods**, which compare the clustering against the group truth and measure. If the ground truth is unavailable, we can use **intrinsic methods**, which evaluate the goodness of a clustering by considering how well the clusters are separated. Ground truth can be considered as supervision in the form of "cluster labels." Hence, extrinsic methods are also known as *supervised methods*, while intrinsic methods are *unsupervised methods*.

Let's have a look at simple methods from each category.

Extrinsic Methods

When the ground truth is available, we can compare it with a clustering to assess the clustering. Thus, the core task in extrinsic methods is to assign a score, $Q(\mathcal{C}, \mathcal{C}_g)$, to a clustering, $\mathcal{C}$, given the ground truth, $\mathcal{C}_g$. Whether an extrinsic method is effective largely depends on the measure, Q, it uses.

In general, a measure Q on clustering quality is effective if it satisfies the following four essential criteria:

- **Cluster homogeneity.** This requires that the more pure the clusters in a clustering are, the better the clustering. Suppose that ground truth says that the objects in a data set, D, can belong to categories $L_1, \ldots, L_n$. Consider clustering, $\mathcal{C}_1$, wherein a cluster $C \in \mathcal{C}_1$ contains objects from two categories L_i, L_j $(1 \leq i < j \leq n)$. Also consider clustering $\mathcal{C}_2$, which is identical to $\mathcal{C}_1$ except that C_2 is split into two clusters containing the objects in L_i and L_j, respectively. A clustering quality measure, Q, respecting cluster homogeneity should give a higher score to $\mathcal{C}_2$ than $\mathcal{C}_1$, that is, $Q(\mathcal{C}_2,\mathcal{C}_g) > Q(\mathcal{C}_1,\mathcal{C}_g)$.

- **Cluster completeness.** This is the counterpart of cluster homogeneity. Cluster completeness requires that for a clustering, if any two objects belong to the same category according to ground truth, then they should be assigned to the same cluster. Cluster completeness requires that a clustering should assign objects belonging to the same category (according to ground truth) to the same cluster. Consider clustering $\mathcal{C}_1$, which contains clusters C_1 and C_2, of which the members belong to the same category according to ground truth. Let clustering $\mathcal{C}_2$ be identical to $\mathcal{C}_1$ except that C_1 and C_2 are merged into one cluster in $\mathcal{C}_2$. Then, a clustering quality measure, Q, respecting cluster completeness should give a higher score to $\mathcal{C}_2$, that is, $Q(\mathcal{C}_2,\mathcal{C}_g) > Q(\mathcal{C}_1,\mathcal{C}_g)$.

- **Rag bag.** In many practical scenarios, there is often a "rag bag" category containing objects that cannot be merged with other objects. Such a category is often called "miscellaneous," "other," and so on. The rag bag criterion states that putting a heterogeneous object into a pure cluster should be penalized more than putting it into a rag bag. Consider a clustering $\mathcal{C}_1$ and a cluster $C \in \mathcal{C}_1$ such that all objects in C except for one, denoted by $\boldsymbol{o}$, belong to the same category according to ground truth. Consider a clustering $\mathcal{C}_2$ identical to $\mathcal{C}_1$ except that $\boldsymbol{o}$ is assigned to a cluster $C' \neq C$ in $\mathcal{C}_2$ such that C' contains objects from various categories according to ground truth, and thus is noisy. In other words, C' in $\mathcal{C}_2$ is a rag bag. Then, a clustering quality measure Q respecting the rag bag criterion should give a higher score to $\mathcal{C}_2$, that is, $Q(\mathcal{C}_2,\mathcal{C}_g) > Q(\mathcal{C}_1,\mathcal{C}_g)$.

- **Small cluster preservation.** If a small category is split into small pieces in a clustering, those small pieces may likely become noise and thus the small category cannot be discovered from the clustering. The small cluster preservation criterion states that splitting a small category into pieces is more harmful than splitting a large category into pieces. Consider an extreme case. Let D be a data set of $n+2$ objects such that, according to ground truth, n objects, denoted by $\boldsymbol{o}_1, \ldots, \boldsymbol{o}_n$, belong to one category and the other two objects, denoted by $\boldsymbol{o}_{n+1}, \boldsymbol{o}_{n+2}$, belong to another category. Suppose clustering $\mathcal{C}_1$ has three clusters, $C_1 = \{\boldsymbol{o}_1, \ldots, \boldsymbol{o}_n\}$, $C_2 = \{\boldsymbol{o}_{n+1}\}$, and $C_3 = \{\boldsymbol{o}_{n+2}\}$. Let clustering $\mathcal{C}_2$ have three clusters, too, namely $C_1 = \{\boldsymbol{o}_1, \ldots, \boldsymbol{o}_{n-1}\}$, $C_2 = \{\boldsymbol{o}_n\}$, and $C_3 = \{\boldsymbol{o}_{n+1}, \boldsymbol{o}_{n+2}\}$. In other words, $\mathcal{C}_1$ splits the small category and $\mathcal{C}_2$ splits the big category. A clustering quality measure Q preserving small clusters should give a higher score to $\mathcal{C}_2$, that is, $Q(\mathcal{C}_2,\mathcal{C}_g) > Q(\mathcal{C}_1,\mathcal{C}_g)$.

Many clustering quality measures satisfy some of these four criteria. Here, we introduce the *BCubed precision* and *recall* metrics, which satisfy all four criteria.

BCubed evaluates the precision and recall for every object in a clustering on a given data set according to ground truth. The precision of an object indicates how many other objects in the same cluster belong to the same category as the object. The recall of an object reflects how many objects of the same category are assigned to the same cluster.

Formally, let $D = \{\boldsymbol{o_1}, \ldots, \boldsymbol{o_n}\}$ be a set of objects, and $\mathcal{C}$ be a clustering on D. Let $L(\boldsymbol{o_i})$ $(1 \leq i \leq n)$ be the category of $\boldsymbol{o_i}$ given by ground truth, and $C(o_i)$ be the *cluster_ID* of $\boldsymbol{o_i}$ in $\mathcal{C}$. Then, for two objects, $\boldsymbol{o_i}$ and $\boldsymbol{o_j}$, $(1 \leq i, j, \leq n, i \neq j)$, the *correctness* of the relation between $\boldsymbol{o_i}$ and $\boldsymbol{o_j}$ in clustering $\mathcal{C}$ is given by

$$\text{Correctness}(\boldsymbol{o_i}, \boldsymbol{o_j}) = \begin{cases} 1 & \text{if } L(\boldsymbol{o_i}) = L(\boldsymbol{o_j}) \Leftrightarrow C(\boldsymbol{o_i}) = C(\boldsymbol{o_j}) \\ 0 & \text{otherwise.} \end{cases} \tag{10.28}$$

BCubed precision is defined as

$$\text{Precision BCubed} = \frac{\displaystyle\sum_{i=1}^{n} \frac{\displaystyle\sum_{\boldsymbol{o_j}: i \neq j, C(\boldsymbol{o_i}) = C(\boldsymbol{o_j})} \text{Correctness}(\boldsymbol{o_i}, \boldsymbol{o_j})}{\| \{\boldsymbol{o_j} | i \neq j, C(\boldsymbol{o_i}) = C(\boldsymbol{o_j})\} \|}}{n}. \tag{10.29}$$

BCubed recall is defined as

$$\text{Recall BCubed} = \frac{\displaystyle\sum_{i=1}^{n} \frac{\displaystyle\sum_{\boldsymbol{o_j}: i \neq j, L(\boldsymbol{o_i}) = L(\boldsymbol{o_j})} \text{Correctness}(\boldsymbol{o_i}, \boldsymbol{o_j})}{\| \{\boldsymbol{o_j} | i \neq j, L(\boldsymbol{o_i}) = L(\boldsymbol{o_j})\} \|}}{n}. \tag{10.30}$$

Intrinsic Methods

When the ground truth of a data set is not available, we have to use an intrinsic method to assess the clustering quality. In general, intrinsic methods evaluate a clustering by examining how well the clusters are separated and how compact the clusters are. Many intrinsic methods have the advantage of a similarity metric between objects in the data set.

The **silhouette coefficient** is such a measure. For a data set, D, of n objects, suppose D is partitioned into k clusters, $C_1, \ldots, C_k$. For each object $\boldsymbol{o} \in D$, we calculate $a(\boldsymbol{o})$ as the average distance between $\boldsymbol{o}$ and all other objects in the cluster to which $\boldsymbol{o}$ belongs. Similarly, $b(\boldsymbol{o})$ is the minimum average distance from $\boldsymbol{o}$ to all clusters to which $\boldsymbol{o}$ does not belong. Formally, suppose $\boldsymbol{o} \in C_i$ $(1 \leq i \leq k)$; then

$$a(\boldsymbol{o}) = \frac{\sum_{\boldsymbol{o'} \in C_i, \boldsymbol{o} \neq \boldsymbol{o'}} dist(\boldsymbol{o}, \boldsymbol{o'})}{|C_i| - 1} \tag{10.31}$$

and

$$b(\boldsymbol{o}) = \min_{C_j:1\le j\le k, j\ne i} \left\{ \frac{\sum_{\boldsymbol{o}' \in C_j} dist(\boldsymbol{o}, \boldsymbol{o}')}{|C_j|} \right\}. \tag{10.32}$$

The **silhouette coefficient** of ***o*** is then defined as

$$s(\boldsymbol{o}) = \frac{b(\boldsymbol{o}) - a(\boldsymbol{o})}{\max\{a(\boldsymbol{o}), b(\boldsymbol{o})\}}. \tag{10.33}$$

The value of the silhouette coefficient is between -1 and 1. The value of $\boldsymbol{a(o)}$ reflects the compactness of the cluster to which ***o*** belongs. The smaller the value, the more compact the cluster. The value of $b(\boldsymbol{o})$ captures the degree to which ***o*** is separated from other clusters. The larger $b(\boldsymbol{o})$ is, the more separated ***o*** is from other clusters. Therefore, when the silhouette coefficient value of ***o*** approaches 1, the cluster containing ***o*** is compact and ***o*** is far away from other clusters, which is the preferable case. However, when the silhouette coefficient value is negative (i.e., $b(\boldsymbol{o}) < \mathrm{a}(\boldsymbol{o})$), this means that, in expectation, ***o*** is closer to the objects in another cluster than to the objects in the same cluster as ***o***. In many cases, this is a bad situation and should be avoided.

To measure a cluster's fitness within a clustering, we can compute the average silhouette coefficient value of all objects in the cluster. To measure the quality of a clustering, we can use the average silhouette coefficient value of all objects in the data set. The silhouette coefficient and other intrinsic measures can also be used in the elbow method to heuristically derive the number of clusters in a data set by replacing the sum of within-cluster variances.

10.7 Summary

- A **cluster** is a collection of data objects that are *similar* to one another within the same cluster and are *dissimilar* to the objects in other clusters. The process of grouping a set of physical or abstract objects into classes of *similar* objects is called **clustering**.

- Cluster analysis has extensive **applications**, including business intelligence, image pattern recognition, Web search, biology, and security. Cluster analysis can be used as a standalone data mining tool to gain insight into the data distribution, or as a preprocessing step for other data mining algorithms operating on the detected clusters.

- Clustering is a dynamic field of research in data mining. It is related to **unsupervised learning** in machine learning.

- Clustering is a challenging field. Typical **requirements** of it include scalability, the ability to deal with different types of data and attributes, the discovery of clusters in arbitrary shape, minimal requirements for domain knowledge to determine input parameters, the ability to deal with noisy data, incremental clustering and insensitivity to input order, the capability of clustering high-dimensionality data, constraint-based clustering, as well as interpretability and usability.

- Many clustering algorithms have been developed. These can be categorized from several **orthogonal aspects** such as those regarding partitioning criteria, separation of clusters, similarity measures used, and clustering space. This chapter discusses major fundamental clustering methods of the following categories: *partitioning methods, hierarchical methods, density-based methods*, and *grid-based methods*. Some algorithms may belong to more than one category.
- A **partitioning method** first creates an initial set of *k* partitions, where parameter *k* is the number of partitions to construct. It then uses an *iterative relocation technique* that attempts to improve the partitioning by moving objects from one group to another. Typical partitioning methods include *k*-means, *k*-medoids, and CLARANS.
- A **hierarchical method** creates a hierarchical decomposition of the given set of data objects. The method can be classified as being either *agglomerative* (*bottom-up*) or *divisive* (*top-down*), based on how the hierarchical decomposition is formed. To compensate for the rigidity of *merge* or *split*, the quality of hierarchical agglomeration can be improved by analyzing object linkages at each hierarchical partitioning (e.g., in Chameleon), or by first performing *microclustering* (that is, grouping objects into "microclusters") and then operating on the microclusters with other clustering techniques such as iterative relocation (as in BIRCH).
- A **density-based method** clusters objects based on the notion of density. It grows clusters either according to the density of neighborhood objects (e.g., in DBSCAN) or according to a density function (e.g., in DENCLUE). OPTICS is a density-based method that generates an augmented ordering of the data's clustering structure.
- A **grid-based method** first quantizes the object space into a finite number of cells that form a grid structure, and then performs clustering on the grid structure. STING is a typical example of a grid-based method based on statistical information stored in grid cells. CLIQUE is a grid-based and subspace clustering algorithm.
- **Clustering evaluation** assesses the feasibility of clustering analysis on a data set and the quality of the results generated by a clustering method. The tasks include assessing clustering tendency, determining the number of clusters, and measuring clustering quality.

10.8 Exercises

10.1 Briefly describe and give examples of each of the following approaches to clustering: *partitioning* methods, *hierarchical* methods, *density-based* methods, and *grid-based* methods.

10.2 Suppose that the data mining task is to cluster points (with (x,y) representing location) into three clusters, where the points are

$$A_1(2,10), A_2(2,5), A_3(8,4), B_1(5,8), B_2(7,5), B_3(6,4), C_1(1,2), C_2(4,9).$$

The distance function is Euclidean distance. Suppose initially we assign A_1, B_1, and C_1 as the center of each cluster, respectively. Use the *k-means* algorithm to show *only*

(a) The three cluster centers after the first round of execution.

(b) The final three clusters.

10.3 Use an example to show why the k-means algorithm may not find the global optimum, that is, optimizing the within-cluster variation.

10.4 For the k-means algorithm, it is interesting to note that by choosing the initial cluster centers carefully, we may be able to not only speed up the algorithm's convergence, but also guarantee the quality of the final clustering. The ***k*-means++** algorithm is a variant of k-means, which chooses the initial centers as follows. First, it selects one center uniformly at random from the objects in the data set. Iteratively, for each object $\boldsymbol{p}$ other than the chosen center, it chooses an object as the new center. This object is chosen at random with probability proportional to $dist(\boldsymbol{p})^2$, where $dist(\boldsymbol{p})$ is the distance from $\boldsymbol{p}$ to the closest center that has already been chosen. The iteration continues until k centers are selected.

Explain why this method will not only speed up the convergence of the k-means algorithm, but also guarantee the quality of the final clustering results.

10.5 Provide the pseudocode of the object reassignment step of the PAM algorithm.

10.6 Both *k-means* and *k-medoids* algorithms can perform effective clustering.

(a) Illustrate the strength and weakness of *k-means* in comparison with *k-medoids*.

(b) Illustrate the strength and weakness of these schemes in comparison with a hierarchical clustering scheme (e.g., AGNES).

10.7 Prove that in DBSCAN, the density-connectedness is an equivalence relation.

10.8 Prove that in DBSCAN, for a fixed *MinPts* value and two neighborhood thresholds, $\epsilon_1 < \epsilon_2$, a cluster C with respect to ϵ_1 and *MinPts* must be a subset of a cluster C' with respect to ϵ_2 and *MinPts*.

10.9 Provide the pseudocode of the OPTICS algorithm.

10.10 Why is it that BIRCH encounters difficulties in finding clusters of arbitrary shape but OPTICS does not? Propose modifications to BIRCH to help it find clusters of arbitrary shape.

10.11 Provide the pseudocode of the step in CLIQUE that finds dense cells in all subspaces.

10.12 Present conditions under which density-based clustering is more suitable than partitioning-based clustering and hierarchical clustering. Give application examples to support your argument.

10.13 Give an example of how specific clustering methods can be *integrated*, for example, where one clustering algorithm is used as a preprocessing step for another. In addition, provide reasoning as to why the integration of two methods may sometimes lead to improved clustering quality and efficiency.

10.14 Clustering is recognized as an important data mining task with broad applications. Give one application example for each of the following cases:

(a) An application that uses clustering as a major data mining function.

(b) An application that uses clustering as a preprocessing tool for data preparation for other data mining tasks.

10.15 Data cubes and multidimensional databases contain nominal, ordinal, and numeric data in hierarchical or aggregate forms. Based on what you have learned about the clustering methods, design a clustering method that finds clusters in large data cubes effectively and efficiently.

10.16 Describe each of the following clustering algorithms in terms of the following criteria: (1) shapes of clusters that can be determined; (2) input parameters that must be specified; and (3) limitations.

(a) *k*-means

(b) *k*-medoids

(c) CLARA

(d) BIRCH

(e) CHAMELEON

(f) DBSCAN

10.17 Human eyes are fast and effective at judging the quality of clustering methods for 2-D data. Can you design a data visualization method that may help humans visualize data clusters and judge the clustering quality for 3-D data? What about for even higher-dimensional data?

10.18 Suppose that you are to allocate a number of automatic teller machines (ATMs) in a given region so as to satisfy a number of constraints. Households or workplaces may be clustered so that typically one ATM is assigned per cluster. The clustering, however, may be constrained by two factors: (1) obstacle objects (i.e., there are bridges, rivers, and highways that can affect ATM accessibility), and (2) additional user-specified constraints such as that each ATM should serve at least 10,000 households. How can a clustering algorithm such as *k*-means be modified for quality clustering under *both* constraints?

10.19 For *constraint-based clustering*, aside from having the minimum number of customers in each cluster (for ATM allocation) as a constraint, there can be many other kinds of constraints. For example, a constraint could be in the form of the maximum number of customers per cluster, average income of customers per cluster, maximum distance between every two clusters, and so on. Categorize the kinds of constraints that can be imposed on the clusters produced and discuss how to perform clustering efficiently under such kinds of constraints.

10.20 Design a *privacy-preserving clustering* method so that a data owner would be able to ask a third party to mine the data for quality clustering without worrying about the potential inappropriate disclosure of certain private or sensitive information stored in the data.

10.21 Show that BCubed metrics satisfy the four essential requirements for extrinsic clustering evaluation methods.

10.9 Bibliographic Notes

Clustering has been extensively studied for over 40 years and across many disciplines due to its broad applications. Most books on pattern classification and machine learning contain chapters on cluster analysis or unsupervised learning. Several textbooks are dedicated to the methods of cluster analysis, including Hartigan [Har75]; Jain and Dubes [JD88]; Kaufman and Rousseeuw [KR90]; and Arabie, Hubert, and De Sorte [AHS96]. There are also many survey articles on different aspects of clustering methods. Recent ones include Jain, Murty, and Flynn [JMF99]; Parsons, Haque, and Liu [PHL04]; and Jain [Jai10].

For partitioning methods, the k-means algorithm was first introduced by Lloyd [Llo57], and then by MacQueen [Mac67]. Arthur and Vassilvitskii [AV07] presented the k-means++ algorithm. A filtering algorithm, which uses a spatial hierarchical data index to speed up the computation of cluster means, is given in Kanungo, Mount, Netanyahu, et al. [KMN$^+$02].

The k-medoids algorithms of PAM and CLARA were proposed by Kaufman and Rousseeuw [KR90]. The k-modes (for clustering nominal data) and k-prototypes (for clustering hybrid data) algorithms were proposed by Huang [Hua98]. The k-modes clustering algorithm was also proposed independently by Chaturvedi, Green, and Carroll [CGC94, CGC01]. The CLARANS algorithm was proposed by Ng and Han [NH94]. Ester, Kriegel, and Xu [EKX95] proposed techniques for further improvement of the performance of CLARANS using efficient spatial access methods such as R$*$-tree and focusing techniques. A k-means-based scalable clustering algorithm was proposed by Bradley, Fayyad, and Reina [BFR98].

An early survey of agglomerative hierarchical clustering algorithms was conducted by Day and Edelsbrunner [DE84]. Agglomerative hierarchical clustering, such as AGNES, and divisive hierarchical clustering, such as DIANA, were introduced by Kaufman and Rousseeuw [KR90]. An interesting direction for improving the clustering quality of hierarchical clustering methods is to integrate hierarchical clustering with distance-based iterative relocation or other nonhierarchical clustering methods. For example, BIRCH, by Zhang, Ramakrishnan, and Livny [ZRL96], first performs hierarchical clustering with a CF-tree before applying other techniques. Hierarchical clustering can also be performed by sophisticated linkage analysis, transformation, or nearest-neighbor analysis, such as CURE by Guha, Rastogi, and Shim [GRS98]; ROCK (for clustering nominal attributes) by Guha, Rastogi, and Shim [GRS99]; and Chameleon by Karypis, Han, and Kumar [KHK99].

A probabilistic hierarchical clustering framework following normal linkage algorithms and using probabilistic models to define cluster similarity was developed by Friedman [Fri03] and Heller and Ghahramani [HG05].

For density-based clustering methods, DBSCAN was proposed by Ester, Kriegel, Sander, and Xu [EKSX96]. Ankerst, Breunig, Kriegel, and Sander [ABKS99] developed OPTICS, a cluster-ordering method that facilitates density-based clustering without worrying about parameter specification. The DENCLUE algorithm, based on a set of density distribution functions, was proposed by Hinneburg and Keim [HK98]. Hinneburg and Gabriel [HG07] developed DENCLUE 2.0, which includes a new hill-climbing procedure for Gaussian kernels that adjusts the step size automatically.

STING, a grid-based multiresolution approach that collects statistical information in grid cells, was proposed by Wang, Yang, and Muntz [WYM97]. WaveCluster, developed by Sheikholeslami, Chatterjee, and Zhang [SCZ98], is a multiresolution clustering approach that transforms the original feature space by wavelet transform.

Scalable methods for clustering nominal data were studied by Gibson, Kleinberg, and Raghavan [GKR98]; Guha, Rastogi, and Shim [GRS99]; and Ganti, Gehrke, and Ramakrishnan [GGR99]. There are also many other clustering paradigms. For example, fuzzy clustering methods are discussed in Kaufman and Rousseeuw [KR90], Bezdek [Bez81], and Bezdek and Pal [BP92].

For high-dimensional clustering, an Apriori-based dimension-growth subspace clustering algorithm called CLIQUE was proposed by Agrawal, Gehrke, Gunopulos, and Raghavan [AGGR98]. It integrates density-based and grid-based clustering methods.

Recent studies have proceeded to clustering stream data Babcock, Badu, Datar, et al. [BBD$^+$02]. A *k*-median-based data stream clustering algorithm was proposed by Guha, Mishra, Motwani, and O'Callaghan [GMMO00] and by O'Callaghan et al. [OMM$^+$02]. A method for clustering evolving data streams was proposed by Aggarwal, Han, Wang, and Yu [AHWY03]. A framework for projected clustering of high-dimensional data streams was proposed by Aggarwal, Han, Wang, and Yu [AHWY04a].

Clustering evaluation is discussed in a few monographs and survey articles such as Jain and Dubes [JD88] and Halkidi, Batistakis, and Vazirgiannis [HBV01]. The extrinsic methods for clustering quality evaluation are extensively explored. Some recent studies include Meilă [Mei03, Mei05] and Amigó, Gonzalo, Artiles, and Verdejo [AGAV09]. The four essential criteria introduced in this chapter are formulated in Amigó, Gonzalo, Artiles, and Verdejo [AGAV09], while some individual criteria were also mentioned earlier, for example, in Meilă [Mei03] and Rosenberg and Hirschberg [RH07]. Bagga and Baldwin [BB98] introduced the BCubed metrics. The silhouette coefficient is described in Kaufman and Rousseeuw [KR90].

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11 Advanced Cluster Analysis

You learned the fundamentals of cluster analysis in Chapter 10. In this chapter, we discuss advanced topics of cluster analysis. Specifically, we investigate four major perspectives:

- **Probabilistic model-based clustering**: Section 11.1 introduces a general framework and a method for deriving clusters where each object is assigned a probability of belonging to a cluster. Probabilistic model-based clustering is widely used in many data mining applications such as text mining.
- **Clustering high-dimensional data**: When the dimensionality is high, conventional distance measures can be dominated by noise. Section 11.2 introduces fundamental methods for cluster analysis on high-dimensional data.
- **Clustering graph and network data**: Graph and network data are increasingly popular in applications such as online social networks, the World Wide Web, and digital libraries. In Section 11.3, you will study the key issues in clustering graph and network data, including similarity measurement and clustering methods.
- **Clustering with constraints**: In our discussion so far, we do not assume any constraints in clustering. In some applications, however, various constraints may exist. These constraints may rise from background knowledge or spatial distribution of the objects. You will learn how to conduct cluster analysis with different kinds of constraints in Section 11.4.

By the end of this chapter, you will have a good grasp of the issues and techniques regarding advanced cluster analysis.

11.1 Probabilistic Model-Based Clustering

In all the cluster analysis methods we have discussed so far, each data object can be assigned to only one of a number of clusters. This cluster assignment rule is required in some applications such as assigning customers to marketing managers. However, in other applications, this rigid requirement may not be desirable. In this section, we demonstrate the need for fuzzy or flexible cluster assignment in some applications, and introduce a general method to compute probabilistic clusters and assignments.

"In what situations may a data object belong to more than one cluster?" Consider Example 11.1.

Example 11.1 **Clustering product reviews.** *AllElectronics* has an online store, where customers not only purchase online, but also create reviews of products. Not every product receives reviews; instead, some products may have many reviews, while many others have none or only a few. Moreover, a review may involve multiple products. Thus, as the review editor of *AllElectronics*, your task is to cluster the reviews.

Ideally, a cluster is about a *topic*, for example, a group of products, services, or issues that are highly related. Assigning a review to one cluster exclusively would not work well for your task. Suppose there is a cluster for "cameras and camcorders" and another for "computers." What if a review talks about the compatibility between a camcorder and a computer? The review relates to both clusters; however, it does not exclusively belong to either cluster.

You would like to use a clustering method that allows a review to belong to more than one cluster if the review indeed involves more than one topic. To reflect the strength that a review belongs to a cluster, you want the assignment of a review to a cluster to carry a weight representing the partial membership. ■

The scenario where an object may belong to multiple clusters occurs often in many applications. This is illustrated in Example 11.2.

Example 11.2 **Clustering to study user search intent**. The *AllElectronics* online store records all customer browsing and purchasing behavior in a log. An important data mining task is to use the log data to categorize and understand *user search intent*. For example, consider a user *session* (a short period in which a user interacts with the online store). Is the user searching for a product, making comparisons among different products, or looking for customer support information? Clustering analysis helps here because it is difficult to predefine user behavior patterns thoroughly. A cluster that contains similar user browsing trajectories may represent similar user behavior.

However, not every session belongs to only one cluster. For example, suppose user sessions involving the purchase of digital cameras form one cluster, and user sessions that compare laptop computers form another cluster. What if a user in one session makes an order for a digital camera, and at the same time compares several laptop computers? Such a session should belong to both clusters to some extent. ■

In this section, we systematically study the theme of clustering that allows an object to belong to more than one cluster. We start with the notion of fuzzy clusters in Section 11.1.1. We then generalize the concept to probabilistic model-based clusters in Section 11.1.2. In Section 11.1.3, we introduce the expectation-maximization algorithm, a general framework for mining such clusters.

11.1.1 Fuzzy Clusters

Given a set of objects, $X = \{x_1, \ldots, x_n\}$, a **fuzzy set** S is a subset of X that allows each object in X to have a membership degree between 0 and 1. Formally, a fuzzy set, S, can be modeled as a function, $F_S{:}X \rightarrow [0,1]$.

Example 11.3 **Fuzzy set.** The more digital camera units that are sold, the more popular the camera is. In *AllElectronics*, we can use the following formula to compute the degree of popularity of a digital camera, o, given the sales of o:

$$pop(o) = \begin{cases} 1 & \text{if 1000 or more units of } o \text{ are sold} \\ \frac{i}{1000} & \text{if } i \ (i < 1000) \text{ units of } o \text{ are sold.} \end{cases} \tag{11.1}$$

Function $pop()$ defines a fuzzy set of popular digital cameras. For example, suppose the sales of digital cameras at *AllElectronics* are as shown in Table 11.1. The fuzzy set of popular digital cameras is $\{A(0.05), B(1), C(0.86), D(0.27)\}$, where the degrees of membership are written in parentheses. ■

We can apply the fuzzy set idea on clusters. That is, given a set of objects, a cluster is a fuzzy set of objects. Such a cluster is called a fuzzy cluster. Consequently, a clustering contains multiple *fuzzy clusters*.

Formally, given a set of objects, $o_1, \ldots, o_n$, a **fuzzy clustering** of k **fuzzy clusters**, $C_1, \ldots, C_k$, can be represented using a **partition matrix**, $M = [w_{ij}]$ $(1 \leq i \leq n, 1 \leq j \leq k)$, where w_{ij} is the membership degree of o_i in fuzzy cluster C_j. The partition matrix should satisfy the following three requirements:

- For each object, o_i, and cluster, C_j, $0 \leq w_{ij} \leq 1$. This requirement enforces that a fuzzy cluster is a fuzzy set.
- For each object, o_i, $\sum_{j=1}^{k} w_{ij} = 1$. This requirement ensures that every object participates in the clustering equivalently.

Table 11.1 Set of Digital Cameras and Their Sales at *AllElectronics*

Camera	*Sales (units)*
A	50
B	1320
C	860
D	270

- For each cluster, C_j, $0 < \sum_{i=1}^{n} w_{ij} < n$. This requirement ensures that for every cluster, there is at least one object for which the membership value is nonzero.

Example 11.4 **Fuzzy clusters.** Suppose the *AllElectronics* online store has six reviews. The keywords contained in these reviews are listed in Table 11.2.

We can group the reviews into two fuzzy clusters, C_1 and C_2. C_1 is for "digital camera" and "lens," and C_2 is for "computer." The partition matrix is

$$M = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ \frac{2}{3} & \frac{1}{3} \\ 0 & 1 \\ 0 & 1 \end{bmatrix}.$$

Here, we use the keywords "digital camera" and "lens" as the features of cluster C_1, and "computer" as the feature of cluster C_2. For review, R_i, and cluster, C_j $(1 \le i \le 6, 1 \le j \le 2)$, w_{ij} is defined as

$$w_{ij} = \frac{|R_i \cap C_j|}{|R_i \cap (C_1 \cup C_2)|} = \frac{|R_i \cap C_j|}{|R_i \cap \{\textit{digital camera, lens, computer}\}|}.$$

In this fuzzy clustering, review R_4 belongs to clusters C_1 and C_2 with membership degrees $\frac{2}{3}$ and $\frac{1}{3}$, respectively. ■

"How can we evaluate how well a fuzzy clustering describes a data set?" Consider a set of objects, $o_1, \ldots, o_n$, and a fuzzy clustering $\mathcal{C}$ of k clusters, $C_1, \ldots, C_k$. Let $M = [w_{ij}]$ $(1 \le i \le n, 1 \le j \le k)$ be the partition matrix. Let $c_1, \ldots, c_k$ be the *centers* of clusters $C_1, \ldots, C_k$, respectively. Here, a center can be defined either as the mean or the medoid, or in other ways specific to the application.

As discussed in Chapter 10, the distance or similarity between an object and the center of the cluster to which the object is assigned can be used to measure how well the

Table 11.2 Set of Reviews and the Keywords Used

Review_ID	*Keywords*
R_1	digital camera, lens
R_2	digital camera
R_3	lens
R_4	digital camera, lens, computer
R_5	computer, CPU
R_6	computer, computer game

object belongs to the cluster. This idea can be extended to fuzzy clustering. For any object, o_i, and cluster, C_j, if $w_{ij} > 0$, then $dist(o_i, c_j)$ measures how well o_i is represented by c_j, and thus belongs to cluster C_j. Because an object can participate in more than one cluster, the sum of distances to the corresponding cluster centers weighted by the degrees of membership captures how well the object fits the clustering.

Formally, for an object o_i, the **sum of the squared error** (SSE) is given by

$$\text{SSE}(o_i) = \sum_{j=1}^{k} w_{ij}^p \, dist(o_i, c_j)^2, \tag{11.2}$$

where the parameter $p (p \geq 1)$ controls the influence of the degrees of membership. The larger the value of p, the larger the influence of the degrees of membership. Orthogonally, the SSE for a cluster, C_j, is

$$\text{SSE}(C_j) = \sum_{i=1}^{n} w_{ij}^p \, dist(o_i, c_j)^2. \tag{11.3}$$

Finally, the SSE of the clustering is defined as

$$\text{SSE}(\mathcal{C}) = \sum_{i=1}^{n} \sum_{j=1}^{k} w_{ij}^p \, dist(o_i, c_j)^2. \tag{11.4}$$

The SSE can be used to measure how well a fuzzy clustering fits a data set.

Fuzzy clustering is also called *soft clustering* because it allows an object to belong to more than one cluster. It is easy to see that traditional (rigid) clustering, which enforces each object to belong to only one cluster exclusively, is a special case of fuzzy clustering. We defer the discussion of how to compute fuzzy clustering to Section 11.1.3.

11.1.2 Probabilistic Model-Based Clusters

"Fuzzy clusters (Section 11.1.1) provide the flexibility of allowing an object to participate in multiple clusters. Is there a general framework to specify clusterings where objects may participate in multiple clusters in a probabilistic way?" In this section, we introduce the general notion of probabilistic model-based clusters to answer this question.

As discussed in Chapter 10, we conduct cluster analysis on a data set because we assume that the objects in the data set in fact belong to different inherent categories. Recall that clustering tendency analysis (Section 10.6.1) can be used to examine whether a data set contains objects that may lead to meaningful clusters. Here, the inherent categories hidden in the data are *latent*, which means they cannot be directly observed. Instead, we have to infer them using the data observed. For example, the topics hidden in a set of reviews in the *AllElectronics* online store are latent because one cannot read the topics directly. However, the topics can be inferred from the reviews because each review is about one or multiple topics.

Therefore, the goal of cluster analysis is to find hidden categories. A data set that is the subject of cluster analysis can be regarded as a sample of the possible instances of the hidden categories, but without any category labels. The clusters derived from cluster analysis are inferred using the data set, and are designed to approach the hidden categories.

Statistically, we can assume that a hidden category is a distribution over the data space, which can be mathematically represented using a probability density function (or distribution function). We call such a hidden category a *probabilistic cluster*. For a probabilistic cluster, C, its probability density function, f, and a point, o, in the data space, $f(o)$ is the relative likelihood that an instance of C appears at o.

Example 11.5 **Probabilistic clusters**. Suppose the digital cameras sold by *AllElectronics* can be divided into two categories: C_1, a consumer line (e.g., point-and-shoot cameras), and C_2, a professional line (e.g., single-lens reflex cameras). Their respective probability density functions, f_1 and f_2, are shown in Figure 11.1 with respect to the attribute *price*.

For a price value of, say, \$1000, $f_1(1000)$ is the relative likelihood that the price of a consumer-line camera is \$1000. Similarly, $f_2(1000)$ is the relative likelihood that the price of a professional-line camera is \$1000.

The probability density functions, f_1 and f_2, cannot be observed directly. Instead, *AllElectronics* can only infer these distributions by analyzing the prices of the digital cameras it sells. Moreover, a camera often does not come with a well-determined category (e.g., "consumer line" or "professional line"). Instead, such categories are typically based on user background knowledge and can vary. For example, a camera in the *prosumer* segment may be regarded at the high end of the consumer line by some customers, and the low end of the professional line by others.

As an analyst at *AllElectronics*, you can consider each category as a probabilistic cluster, and conduct cluster analysis on the price of cameras to approach these categories. ■

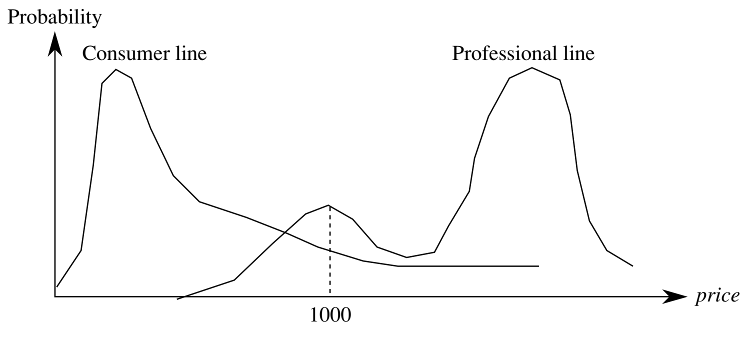


Figure 11.1 The probability density functions of two probabilistic clusters.

Suppose we want to find k probabilistic clusters, $C_1, \ldots, C_k$, through cluster analysis. For a data set, D, of n objects, we can regard D as a finite sample of the possible instances of the clusters. Conceptually, we can assume that D is formed as follows. Each cluster, C_j $(1 \leq j \leq k)$, is associated with a probability, ω_j, that some instance is sampled from the cluster. It is often assumed that $\omega_1, \ldots, \omega_k$ are given as part of the problem setting, and that $\sum_{j=1}^{k} \omega_j = 1$, which ensures that all objects are generated by the k clusters. Here, parameter ω_j captures background knowledge about the relative population of cluster C_j.

We then run the following two steps to generate an object in D. The steps are executed n times in total to generate n objects, $o_1, \ldots, o_n$, in D.

1. Choose a cluster, C_j, according to probabilities $\omega_1, \ldots, \omega_k$.
2. Choose an instance of C_j according to its probability density function, f_j.

The data generation process here is the basic assumption in mixture models. Formally, a **mixture model** assumes that a set of observed objects is a mixture of instances from multiple probabilistic clusters. Conceptually, each observed object is generated independently by two steps: first choosing a probabilistic cluster according to the probabilities of the clusters, and then choosing a sample according to the probability density function of the chosen cluster.

Given data set, D, and k, the number of clusters required, the task of *probabilistic model-based cluster analysis* is to infer a set of k probabilistic clusters that is most likely to generate D using this data generation process. An important question remaining is how we can measure the likelihood that a set of k probabilistic clusters and their probabilities will generate an observed data set.

Consider a set, $\boldsymbol{C}$, of k probabilistic clusters, $C_1, \ldots, C_k$, with probability density functions $f_1, \ldots, f_k$, respectively, and their probabilities, $\omega_1, \ldots, \omega_k$. For an object, o, the probability that o is generated by cluster C_j $(1 \leq j \leq k)$ is given by $P(o|C_j) = \omega_j f_j(o)$. Therefore, the probability that o is generated by the set $\boldsymbol{C}$ of clusters is

$$P(o|\boldsymbol{C}) = \sum_{j=1}^{k} \omega_j f_j(o). \tag{11.5}$$

Since the objects are assumed to have been generated independently, for a data set, $D = \{o_1, \ldots, o_n\}$, of n objects, we have

$$P(D|\boldsymbol{C}) = \prod_{i=1}^{n} P(o_i|\boldsymbol{C}) = \prod_{i=1}^{n} \sum_{j=1}^{k} \omega_j f_j(o_i). \tag{11.6}$$

Now, it is clear that the task of probabilistic model-based cluster analysis on a data set, D, is to find a set $\boldsymbol{C}$ of k probabilistic clusters such that $P(D|\boldsymbol{C})$ is maximized. Maximizing $P(D|\boldsymbol{C})$ is often intractable because, in general, the probability density function of a cluster can take an arbitrarily complicated form. To make probabilistic model-based clusters computationally feasible, we often compromise by assuming that the probability density functions are parameterized distributions.

Formally, let $o_1, \ldots, o_n$ be the n observed objects, and $\Theta_1, \ldots, \Theta_k$ be the parameters of the k distributions, denoted by $\mathbf{O} = \{o_1, \ldots, o_n\}$ and $\Theta = \{\Theta_1, \ldots, \Theta_k\}$, respectively. Then, for any object, $o_i \in \mathbf{O}$ $(1 \le i \le n)$, Eq. (11.5) can be rewritten as

$$P(o_i|\Theta) = \sum_{j=1}^{k} \omega_j P_j(o_i|\Theta_j), \tag{11.7}$$

where $P_j(o_i|\Theta_j)$ is the probability that o_i is generated from the jth distribution using parameter Θ_j. Consequently, Eq. (11.6) can be rewritten as

$$P(\mathbf{O}|\Theta) = \prod_{i=1}^{n} \sum_{j=1}^{k} \omega_j P_j(o_i|\Theta_j). \tag{11.8}$$

Using the parameterized probability distribution models, the task of probabilistic model-based cluster analysis is to infer a set of parameters, Θ, that maximizes Eq. (11.8).

Example 11.6 **Univariate Gaussian mixture model.** Let's use univariate Gaussian distributions as an example. That is, we assume that the probability density function of each cluster follows a 1-D Gaussian distribution. Suppose there are k clusters. The two parameters for the probability density function of each cluster are center, μ_j, and standard deviation, σ_j $(1 \le j \le k)$. We denote the parameters as $\Theta_j = (\mu_j, \sigma_j)$ and $\Theta = \{\Theta_1, \ldots, \Theta_k\}$. Let the data set be $\mathbf{O} = \{o_1, \ldots, o_n\}$, where o_i $(1 \le i \le n)$ is a real number. For any point, $o_i \in \mathbf{O}$, we have

$$P(o_i|\Theta_j) = \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i-\mu_j)^2}{2\sigma^2}}. \tag{11.9}$$

Assuming that each cluster has the same probability, that is $\omega_1 = \omega_2 = \cdots = \omega_k = \frac{1}{k}$, and plugging Eq. (11.9) into Eq. (11.7), we have

$$P(o_i|\Theta) = \frac{1}{k} \sum_{j=1}^{k} \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i-\mu_j)^2}{2\sigma^2}}. \tag{11.10}$$

Applying Eq. (11.8), we have

$$P(\mathbf{O}|\Theta) = \frac{1}{k} \prod_{i=1}^{n} \sum_{j=1}^{k} \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i-\mu_j)^2}{2\sigma^2}}. \tag{11.11}$$

The task of probabilistic model-based cluster analysis using a univariate Gaussian mixture model is to infer Θ such that Eq. (11.11) is maximized. ■

11.1.3 Expectation-Maximization Algorithm

"How can we compute fuzzy clusterings and probabilistic model-based clusterings?" In this section, we introduce a principled approach. Let's start with a review of the *k*-means clustering problem and the *k*-means algorithm studied in Chapter 10.

It can easily be shown that *k*-means clustering is a special case of fuzzy clustering (Exercise 11.1). The *k*-means algorithm iterates until the clustering cannot be improved. Each iteration consists of two steps:

The expectation step (E-step): Given the current cluster centers, each object is assigned to the cluster with a center that is closest to the object. Here, an object is expected to belong to the closest cluster.

The maximization step (M-step): Given the cluster assignment, for each cluster, the algorithm adjusts the center so that the sum of the distances from the objects assigned to this cluster and the new center is minimized. That is, the similarity of objects assigned to a cluster is maximized.

We can generalize this two-step method to tackle fuzzy clustering and probabilistic model-based clustering. In general, an **expectation-maximization (EM) algorithm** is a framework that approaches maximum likelihood or maximum a posteriori estimates of parameters in statistical models. In the context of fuzzy or probabilistic model-based clustering, an EM algorithm starts with an initial set of parameters and iterates until the clustering cannot be improved, that is, until the clustering converges or the change is sufficiently small (less than a preset threshold). Each iteration also consists of two steps:

- The **expectation step** assigns objects to clusters according to the current fuzzy clustering or parameters of probabilistic clusters.
- The **maximization step** finds the new clustering or parameters that maximize the SSE in fuzzy clustering (Eq. 11.4) or the expected likelihood in probabilistic model-based clustering.

Example 11.7 **Fuzzy clustering using the EM algorithm.** Consider the six points in Figure 11.2, where the coordinates of the points are also shown. Let's compute two fuzzy clusters using the EM algorithm.

We randomly select two points, say $c_1 = a$ and $c_2 = b$, as the initial centers of the two clusters. The first iteration conducts the expectation step and the maximization step as follows.

In the **E-step**, for each point we calculate its membership degree in each cluster. For any point, o, we assign o to c_1 and c_2 with membership weights

$$\frac{\frac{1}{dist(o,c_1)^2}}{\frac{1}{dist(o,c_1)^2}+\frac{1}{dist(o,c_2)^2}} = \frac{dist(o,c_2)^2}{dist(o,c_1)^2+dist(o,c_2)^2} \text{ and } \frac{dist(o,c_1)^2}{dist(o,c_1)^2+dist(o,c_2)^2},$$

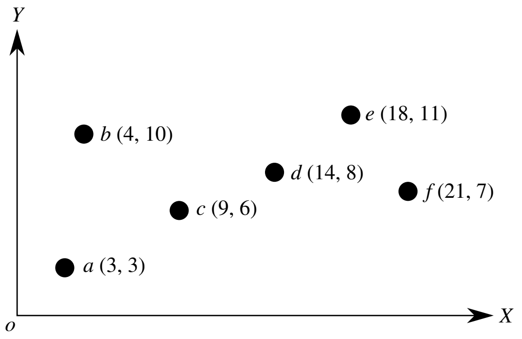


Figure 11.2 Data set for fuzzy clustering.

Table 11.3 Intermediate Results from the First Three Iterations of Example 11.7's EM Algorithm

Iteration	*E-Step*	*M-Step*
1	$M^T = \begin{bmatrix} 1 & 0 & 0.48 & 0.42 & 0.41 & 0.47 \\ 0 & 1 & 0.52 & 0.58 & 0.59 & 0.53 \end{bmatrix}$	$c_1 = (8.47,\ 5.12)$ $c_2 = (10.42,\ 8.99)$
2	$M^T = \begin{bmatrix} 0.73 & 0.49 & 0.91 & 0.26 & 0.33 & 0.42 \\ 0.27 & 0.51 & 0.09 & 0.74 & 0.67 & 0.58 \end{bmatrix}$	$c_1 = (8.51,\ 6.11)$ $c_2 = (14.42,\ 8.69)$
3	$M^T = \begin{bmatrix} 0.80 & 0.76 & 0.99 & 0.02 & 0.14 & 0.23 \\ 0.20 & 0.24 & 0.01 & 0.98 & 0.86 & 0.77 \end{bmatrix}$	$c_1 = (6.40,\ 6.24)$ $c_2 = (16.55,\ 8.64)$

respectively, where $dist(,)$ is the Euclidean distance. The rationale is that, if o is close to c_1 and $dist(o, c_1)$ is small, the membership degree of o with respect to c_1 should be high. We also normalize the membership degrees so that the sum of degrees for an object is equal to 1.

For point a, we have $w_{a,c_1} = 1$ and $w_{a,c_2} = 0$. That is, a exclusively belongs to c_1. For point b, we have $w_{b,c_1} = 0$ and $w_{b,c_2} = 1$. For point c, we have $w_{c,c_1} = \frac{41}{45+41} = 0.48$ and $w_{c,c_2} = \frac{45}{45+41} = 0.52$. The degrees of membership of the other points are shown in the partition matrix in Table 11.3. ■

In the **M-step**, we recalculate the centroids according to the partition matrix, minimizing the SSE given in Eq. (11.4). The new centroid should be adjusted to

$$c_j = \frac{\sum\limits_{\text{each point } o} w_{o,c_j}^2\, o}{\sum\limits_{\text{each point } o} w_{o,c_j}^2}, \tag{11.12}$$

where $j = 1, 2$.

In this example,

$$c_1 = \left(\frac{1^2 \times 3 + 0^2 \times 4 + 0.48^2 \times 9 + 0.42^2 \times 14 + 0.41^2 \times 18 + 0.47^2 \times 21}{1^2 + 0^2 + 0.48^2 + 0.42^2 + 0.41^2 + 0.47^2}, \right.$$

$$\left. \frac{1^2 \times 3 + 0^2 \times 10 + 0.48^2 \times 6 + 0.42^2 \times 8 + 0.41^2 \times 11 + 0.47^2 \times 7}{1^2 + 0^2 + 0.48^2 + 0.42^2 + 0.41^2 + 0.47^2} \right)$$

$$= (8.47, 5.12)$$

and

$$c_2 = \left(\frac{0^2 \times 3 + 1^2 \times 4 + 0.52^2 \times 9 + 0.58^2 \times 14 + 0.59^2 \times 18 + 0.53^2 \times 21}{0^2 + 1^2 + 0.52^2 + 0.58^2 + 0.59^2 + 0.53^2}, \right.$$

$$\left. \frac{0^2 \times 3 + 1^2 \times 10 + 0.52^2 \times 6 + 0.58^2 \times 8 + 0.59^2 \times 11 + 0.53^2 \times 7}{0^2 + 1^2 + 0.52^2 + 0.58^2 + 0.59^2 + 0.53^2} \right)$$

$$= (10.42, 8.99).$$

We repeat the iterations, where each iteration contains an E-step and an M-step. Table 11.3 shows the results from the first three iterations. The algorithm stops when the cluster centers converge or the change is small enough.

"How can we apply the EM algorithm to compute probabilistic model-based clustering?" Let's use a univariate Gaussian mixture model (Example 11.6) to illustrate.

Example 11.8 **Using the EM algorithm for mixture models.** Given a set of objects, $\mathbf{O} = \{o_1, \ldots, o_n\}$, we want to mine a set of parameters, $\Theta = \{\Theta_1, \ldots, \Theta_k\}$, such that $P(\mathbf{O}|\Theta)$ in Eq. (11.11) is maximized, where $\Theta_j = (\mu_j, \sigma_j)$ are the mean and standard deviation, respectively, of the jth univariate Gaussian distribution, $(1 \le j \le k)$.

We can apply the EM algorithm. We assign random values to parameters Θ as the initial values. We then iteratively conduct the E-step and the M-step as follows until the parameters converge or the change is sufficiently small.

In the **E-step**, for each object, $o_i \in \mathbf{O}$ $(1 \le i \le n)$, we calculate the probability that o_i belongs to each distribution, that is,

$$P(\Theta_j | o_i, \Theta) = \frac{P(o_i|\Theta_j)}{\sum_{l=1}^{k} P(o_i|\Theta_l)}. \tag{11.13}$$

In the **M-step**, we adjust the parameters Θ so that the expected likelihood $P(\mathbf{O}|\Theta)$ in Eq. (11.11) is maximized. This can be achieved by setting

$$\mu_j = \frac{1}{k} \sum_{i=1}^{n} o_i \frac{P(\Theta_j|o_i, \Theta)}{\sum_{l=1}^{n} P(\Theta_j|o_l, \Theta)} = \frac{1}{k} \frac{\sum_{i=1}^{n} o_i P(\Theta_j|o_i, \Theta)}{\sum_{i=1}^{n} P(\Theta_j|o_i, \Theta)} \tag{11.14}$$

and

$$\sigma_j = \sqrt{\frac{\sum_{i=1}^{n} P(\Theta_j|o_i,\Theta)(o_i - u_j)^2}{\sum_{i=1}^{n} P(\Theta_j|o_i,\Theta)}}. \qquad (11.15)$$

■

In many applications, probabilistic model-based clustering has been shown to be effective because it is more general than partitioning methods and fuzzy clustering methods. A distinct advantage is that appropriate statistical models can be used to capture latent clusters. The EM algorithm is commonly used to handle many learning problems in data mining and statistics due to its simplicity. Note that, in general, the EM algorithm may not converge to the optimal solution. It may instead converge to a local maximum. Many heuristics have been explored to avoid this. For example, we could run the EM process multiple times using different random initial values. Furthermore, the EM algorithm can be very costly if the number of distributions is large or the data set contains very few observed data points.

11.2 Clustering High-Dimensional Data

The clustering methods we have studied so far work well when the dimensionality is not high, that is, having less than 10 attributes. There are, however, important applications of high dimensionality. *"How can we conduct cluster analysis on high-dimensional data?"*

In this section, we study approaches to clustering high-dimensional data. Section 11.2.1 starts with an overview of the major challenges and the approaches used. Methods for high-dimensional data clustering can be divided into two categories: subspace clustering methods (Section 11.2.2) and dimensionality reduction methods (Section 11.2.3).

11.2.1 Clustering High-Dimensional Data: Problems, Challenges, and Major Methodologies

Before we present any specific methods for clustering high-dimensional data, let's first demonstrate the needs of cluster analysis on high-dimensional data using examples. We examine the challenges that call for new methods. We then categorize the major methods according to whether they search for clusters in subspaces of the original space, or whether they create a new lower-dimensionality space and search for clusters there.

In some applications, a data object may be described by 10 or more attributes. Such objects are referred to as a high-dimensional data space.

Example 11.9 **High-dimensional data and clustering.** *AllElectronics* keeps track of the products purchased by every customer. As a customer-relationship manager, you want to cluster customers into groups according to what they purchased from *AllElectronics*.

Table 11.4 Customer Purchase Data

Customer	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	P_9	P_{10}
Ada	1	0	0	0	0	0	0	0	0	0
Bob	0	0	0	0	0	0	0	0	0	1
Cathy	1	0	0	0	1	0	0	0	0	1

The customer purchase data are of very high dimensionality. *AllElectronics* carries tens of thousands of products. Therefore, a customer's purchase profile, which is a vector of the products carried by the company, has tens of thousands of dimensions.

"Are the traditional distance measures, which are frequently used in low-dimensional cluster analysis, also effective on high-dimensional data?" Consider the customers in Table 11.4, where 10 products, $P_1, \ldots, P_{10}$, are used in demonstration. If a customer purchases a product, a 1 is set at the corresponding bit; otherwise, a 0 appears. Let's calculate the Euclidean distances (Eq. 2.16) among Ada, Bob, and Cathy. It is easy to see that

$$dist(\text{Ada}, \text{Bob}) = dist(\text{Bob}, \text{Cathy}) = dist(\text{Ada}, \text{Cathy}) = \sqrt{2}.$$

According to Euclidean distance, the three customers are equivalently similar (or dissimilar) to each other. However, a close look tells us that Ada should be more similar to Cathy than to Bob because Ada and Cathy share one common purchased item, P_1. ■

As shown in Example 11.9, the traditional distance measures can be ineffective on high-dimensional data. Such distance measures may be dominated by the noise in many dimensions. Therefore, clusters in the full, high-dimensional space can be unreliable, and finding such clusters may not be meaningful.

"Then what kinds of clusters are meaningful on high-dimensional data?" For cluster analysis of high-dimensional data, we still want to group similar objects together. However, the data space is often too big and too messy. An additional challenge is that we need to find not only clusters, but, for each cluster, a set of attributes that manifest the cluster. In other words, a cluster on high-dimensional data often is defined using a small set of attributes instead of the full data space. Essentially, clustering high-dimensional data should return groups of objects as clusters (as conventional cluster analysis does), *in addition to*, for each cluster, the set of attributes that characterize the cluster. For example, in Table 11.4, to characterize the similarity between Ada and Cathy, P_1 may be returned as the attribute because Ada and Cathy both purchased P_1.

Clustering high-dimensional data is the search for clusters and the space in which they exist. Thus, there are two major kinds of methods:

- *Subspace clustering approaches* search for clusters existing in subspaces of the given high-dimensional data space, where a subspace is defined using a subset of attributes in the full space. Subspace clustering approaches are discussed in Section 11.2.2.

- *Dimensionality reduction approaches* try to construct a much lower-dimensional space and search for clusters in such a space. Often, a method may construct new dimensions by combining some dimensions from the original data. Dimensionality reduction methods are the topic of Section 11.2.4.

In general, clustering high-dimensional data raises several new challenges in addition to those of conventional clustering:

- A major issue is how to create appropriate models for clusters in high-dimensional data. Unlike conventional clusters in low-dimensional spaces, clusters hidden in high-dimensional data are often significantly smaller. For example, when clustering customer-purchase data, we would not expect many users to have similar purchase patterns. Searching for such small but meaningful clusters is like finding needles in a haystack. As shown before, the conventional distance measures can be ineffective. Instead, we often have to consider various more sophisticated techniques that can model correlations and consistency among objects in subspaces.
- There are typically an exponential number of possible subspaces or dimensionality reduction options, and thus the optimal solutions are often computationally prohibitive. For example, if the original data space has 1000 dimensions, and we want to find clusters of dimensionality 10, then there are $\binom{1000}{10} = 2.63 \times 10^{23}$ possible subspaces.

11.2.2 Subspace Clustering Methods

"How can we find subspace clusters from high-dimensional data?" Many methods have been proposed. They generally can be categorized into three major groups: *subspace search methods*, *correlation-based clustering methods*, and *biclustering methods*.

Subspace Search Methods

A subspace search method searches various subspaces for clusters. Here, a cluster is a subset of objects that are similar to each other in a subspace. The similarity is often captured by conventional measures such as distance or density. For example, the CLIQUE algorithm introduced in Section 10.5.2 is a subspace clustering method. It enumerates subspaces and the clusters in those subspaces in a dimensionality-increasing order, and applies antimonotonicity to prune subspaces in which no cluster may exist.

A major challenge that subspace search methods face is how to search a series of subspaces effectively and efficiently. Generally there are two kinds of strategies:

- *Bottom-up approaches* start from low-dimensional subspaces and search higher-dimensional subspaces only when there may be clusters in those higher-dimensional subspaces. Various pruning techniques are explored to reduce the number of higher-dimensional subspaces that need to be searched. CLIQUE is an example of a bottom-up approach.

- *Top-down approaches* start from the full space and search smaller and smaller subspaces recursively. Top-down approaches are effective only if the *locality assumption* holds, which require that the subspace of a cluster can be determined by the local neighborhood.

Example 11.10 **PROCLUS, a top-down subspace approach.** PROCLUS is a k-medoid-like method that first generates k potential cluster centers for a high-dimensional data set using a sample of the data set. It then refines the subspace clusters iteratively. In each iteration, for each of the current k-medoids, PROCLUS considers the local neighborhood of the medoid in the whole data set, and identifies a subspace for the cluster by minimizing the standard deviation of the distances of the points in the neighborhood to the medoid on each dimension. Once all the subspaces for the medoids are determined, each point in the data set is assigned to the closest medoid according to the corresponding subspace. Clusters and possible outliers are identified. In the next iteration, new medoids replace existing ones if doing so improves the clustering quality. ■

Correlation-Based Clustering Methods

While subspace search methods search for clusters with a similarity that is measured using conventional metrics like distance or density, *correlation-based approaches* can further discover clusters that are defined by advanced correlation models.

Example 11.11 **A correlation-based approach using PCA.** As an example, a *PCA-based approach* first applies PCA (Principal Components Analysis; see Chapter 3) to derive a set of new, uncorrelated dimensions, and then mine clusters in the new space or its subspaces. In addition to PCA, other space transformations may be used, such as the Hough transform or fractal dimensions. ■

For additional details on subspace search methods and correlation-based clustering methods, please refer to the bibliographic notes (Section 11.7).

Biclustering Methods

In some applications, we want to cluster both objects and attributes simultaneously. The resulting clusters are known as *biclusters* and meet four requirements: (1) only a small set of objects participate in a cluster; (2) a cluster only involves a small number of attributes; (3) an object may participate in multiple clusters, or does not participate in any cluster; and (4) an attribute may be involved in multiple clusters, or is not involved in any cluster. Section 11.2.3 discusses biclustering in detail.

11.2.3 Biclustering

In the cluster analysis discussed so far, we cluster objects according to their attribute values. Objects and attributes are not treated in the same way. However, in some applications, objects and attributes are defined in a symmetric way, where data analysis involves searching data matrices for submatrices that show unique patterns as clusters. This kind of clustering technique belongs to the category of biclustering.

This section first introduces two motivating application examples of biclustering—gene expression and recommender systems. You will then learn about the different types of biclusters. Last, we present biclustering methods.

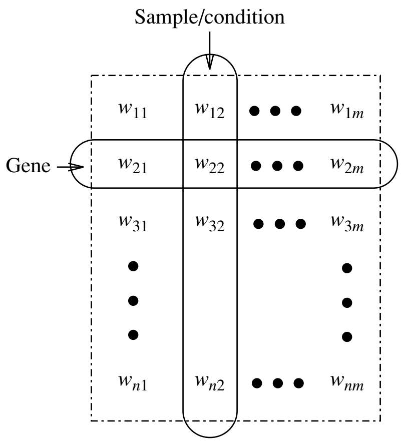
Application Examples

Biclustering techniques were first proposed to address the needs for analyzing gene expression data. A *gene* is a unit of the passing-on of traits from a living organism to its offspring. Typically, a gene resides on a segment of DNA. Genes are critical for all living things because they specify all proteins and functional RNA chains. They hold the information to build and maintain a living organism's cells and pass genetic traits to offspring. Synthesis of a functional gene product, either RNA or protein, relies on the process of gene expression. A *genotype* is the genetic makeup of a cell, an organism, or an individual. *Phenotypes* are observable characteristics of an organism. *Gene expression* is the most fundamental level in genetics in that genotypes cause phenotypes.

Using *DNA chips* (also known as *DNA microarrays*) and other biological engineering techniques, we can measure the expression level of a large number (possibly all) of an organism's genes, in a number of different experimental conditions. Such conditions may correspond to different time points in an experiment or samples from different organs. Roughly speaking, the *gene expression data* or *DNA microarray data* are conceptually a gene-sample/condition matrix, where each row corresponds to one gene, and each column corresponds to one sample or condition. Each element in the matrix is a real number and records the expression level of a gene under a specific condition. Figure 11.3 shows an illustration.

From the clustering viewpoint, an interesting issue is that a gene expression data matrix can be analyzed in two dimensions—the gene dimension and the sample/condition dimension.

- When analyzing in the *gene dimension*, we treat each gene as an object and treat the samples/conditions as attributes. By mining in the gene dimension, we may find patterns shared by multiple genes, or cluster genes into groups. For example, we may find a group of genes that express themselves similarly, which is highly interesting in bioinformatics, such as in finding pathways.
- When analyzing in the *sample/condition dimension*, we treat each sample/condition as an object and treat the genes as attributes. In this way, we may find patterns of samples/conditions, or cluster samples/conditions into groups. For example, we may find the differences in gene expression by comparing a group of tumor samples and nontumor samples.



Sample/condition
Gene
w_{11} w_{12} ••• w_{1m}
w_{21} w_{22} ••• w_{2m}
w_{31} w_{32} ••• w_{3m}
w_{n1} w_{n2} ••• w_{nm}

Figure 11.3 Microarrary data matrix.

Example 11.12 **Gene expression.** Gene expression matrices are popular in bioinformatics research and development. For example, an important task is to classify a new gene using the expression data of the gene and that of other genes in known classes. Symmetrically, we may classify a new sample (e.g., a new patient) using the expression data of the sample and that of samples in known classes (e.g., tumor and nontumor). Such tasks are invaluable in understanding the mechanisms of diseases and in clinical treatment. ■

As can be seen, many gene expression data mining problems are highly related to cluster analysis. However, a challenge here is that, instead of clustering in one dimension (e.g., gene or sample/condition), in many cases we need to cluster in two dimensions simultaneously (e.g., both gene and sample/condition). Moreover, unlike the clustering models we have discussed so far, a cluster in a gene expression data matrix is a *submatrix* and usually has the following characteristics:

- Only a small set of genes participate in the cluster.
- The cluster involves only a small subset of samples/conditions.
- A gene may participate in multiple clusters, or may not participate in any cluster.
- A sample/condition may be involved in multiple clusters, or may not be involved in any cluster.

To find clusters in gene-sample/condition matrices, we need new clustering techniques that meet the following requirements for *biclustering*:

- A cluster of genes is defined using only a subset of samples/conditions.
- A cluster of samples/conditions is defined using only a subset of genes.

- The clusters are neither *exclusive* (e.g., where one gene can participate in multiple clusters) nor *exhaustive* (e.g., where a gene may not participate in any cluster).

Biclustering is useful not only in bioinformatics, but also in other applications as well. Consider recommender systems as an example.

Example 11.13 **Using biclustering for a recommender system.** *AllElectronics* collects data from customers' evaluations of products and uses the data to recommend products to customers. The data can be modeled as a customer-product matrix, where each row represents a customer, and each column represents a product. Each element in the matrix represents a customer's evaluation of a product, which may be a score (e.g., like, like somewhat, not like) or purchase behavior (e.g., buy or not). Figure 11.4 illustrates the structure.

The customer-product matrix can be analyzed in two dimensions: the *customer* dimension and the *product* dimension. Treating each customer as an object and products as attributes, *AllElectronics* can find customer groups that have similar preferences or purchase patterns. Using products as objects and customers as attributes, *AllElectronics* can mine product groups that are similar in customer interest.

Moreover, *AllElectronics* can mine clusters in both customers and products simultaneously. Such a cluster contains a subset of customers and involves a subset of products. For example, *AllElectronics* is highly interested in finding a group of customers who all like the same group of products. Such a cluster is a submatrix in the customer-product matrix, where all elements have a high value. Using such a cluster, *AllElectronics* can make recommendations in two directions. First, the company can recommend products to new customers who are similar to the customers in the cluster. Second, the company can recommend to customers new products that are similar to those involved in the cluster. ■

As with biclusters in a gene expression data matrix, the biclusters in a customer-product matrix usually have the following characteristics:

- Only a small set of customers participate in a cluster.
- A cluster involves only a small subset of products.
- A customer can participate in multiple clusters, or may not participate in any cluster.

$$\begin{array}{lcccc}
 & & \text{Products} & & \\
 & w_{11} & w_{12} & \cdots & w_{1m} \\
\text{Customers} & w_{21} & w_{22} & \cdots & w_{2m} \\
 & \cdots & \cdots & \cdots & \cdots \\
 & w_{n1} & w_{n2} & \cdots & w_{nm}
\end{array}$$

Figure 11.4 Customer–product matrix.

- A product may be involved in multiple clusters, or may not be involved in any cluster.

Biclustering can be applied to customer-product matrices to mine clusters satisfying these requirements.

Types of Biclusters

"How can we model biclusters and mine them?" Let's start with some basic notation. For the sake of simplicity, we will use "genes" and "conditions" to refer to the two dimensions in our discussion. Our discussion can easily be extended to other applications. For example, we can simply replace "genes" and "conditions" by "customers" and "products" to tackle the customer-product biclustering problem.

Let $A = \{a_1, \ldots, a_n\}$ be a set of genes and $B = \{b_1, \ldots, b_m\}$ be a set of conditions. Let $E = [e_{ij}]$ be a gene expression data matrix, that is, a gene-condition matrix, where $1 \leq i \leq n$ and $1 \leq j \leq m$. A submatrix $I \times J$ is defined by a subset $I \subseteq A$ of genes and a subset $J \subseteq B$ of conditions. For example, in the matrix shown in Figure 11.5, $\{a_1, a_{33}, a_{86}\} \times \{b_6, b_{12}, b_{36}, b_{99}\}$ is a submatrix.

A bicluster is a submatrix where genes and conditions follow consistent patterns. We can define different types of biclusters based on such patterns.

- As the simplest case, a submatrix $I \times J$ ($I \subseteq A, J \subseteq B$) is a **bicluster with constant values** if for any $i \in I$ and $j \in J$, $e_{ij} = c$, where c is a constant. For example, the submatrix $\{a_1, a_{33}, a_{86}\} \times \{b_6, b_{12}, b_{36}, b_{99}\}$ in Figure 11.5 is a bicluster with constant values.
- A bicluster is interesting if each row has a constant value, though different rows may have different values. A **bicluster with constant values on rows** is a submatrix $I \times J$ such that for any $i \in I$ and $j \in J$, $e_{ij} = c + \alpha_i$, where α_i is the adjustment for row i. For example, Figure 11.6 shows a bicluster with constant values on rows.

  Symmetrically, a **bicluster with constant values on columns** is a submatrix $I \times J$ such that for any $i \in I$ and $j \in J$, $e_{ij} = c + \beta_j$, where β_j is the adjustment for column j.

	$\cdots$	b_6	$\cdots$	b_{12}	$\cdots$	b_{36}	$\cdots$	b_{99}	$\cdots$
a_1	$\cdots$	60	$\cdots$	60	$\cdots$	60	$\cdots$	60	$\cdots$
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
a_{33}	$\cdots$	60	$\cdots$	60	$\cdots$	60	$\cdots$	60	$\cdots$
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
a_{86}	$\cdots$	60	$\cdots$	60	$\cdots$	60	$\cdots$	60	$\cdots$
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$

Figure 11.5 Gene-condition matrix, a submatrix, and a bicluster.

- More generally, a bicluster is interesting if the rows change in a synchronized way with respect to the columns and vice versa. Mathematically, a **bicluster with coherent values** (also known as **a pattern-based cluster**) is a submatrix $I \times J$ such that for any $i \in I$ and $j \in J$, $e_{ij} = c + \alpha_i + \beta_j$, where α_i and β_j are the adjustment for row i and column j, respectively. For example, Figure 11.7 shows a bicluster with coherent values.

  It can be shown that $I \times J$ is a bicluster with coherent values if and only if for any $i_1, i_2 \in I$ and $j_1, j_2 \in J$, then $e_{i_1 j_1} - e_{i_2 j_1} = e_{i_1 j_2} - e_{i_2 j_2}$. Moreover, instead of using addition, we can define a bicluster with coherent values using multiplication, that is, $e_{ij} = c \cdot (\alpha_i \cdot \beta_j)$. Clearly, biclusters with constant values on rows or columns are special cases of biclusters with coherent values.

- In some applications, we may only be interested in the up- or down-regulated changes across genes or conditions without constraining the exact values. A **bicluster with coherent evolutions on rows** is a submatrix $I \times J$ such that for any $i_1, i_2 \in I$ and $j_1, j_2 \in J$, $(e_{i_1 j_1} - e_{i_1 j_2})(e_{i_2 j_1} - e_{i_2 j_2}) \geq 0$. For example, Figure 11.8 shows a bicluster with coherent evolutions on rows. Symmetrically, we can define biclusters with coherent evolutions on columns.

Next, we study how to mine biclusters.

10	10	10	10	10
20	20	20	20	20
50	50	50	50	50
0	0	0	0	0

Figure 11.6 Bicluster with constant values on rows.

10	50	30	70	20
20	60	40	80	30
50	90	70	110	60
0	40	20	60	10

Figure 11.7 Bicluster with coherent values.

10	50	30	70	20
20	100	50	1000	30
50	100	90	120	80
0	80	20	100	10

Figure 11.8 Bicluster with coherent evolutions on rows.

Biclustering Methods

The previous specification of the types of biclusters only considers ideal cases. In real data sets, such perfect biclusters rarely exist. When they do exist, they are usually very small. Instead, random noise can affect the readings of e_{ij} and thus prevent a bicluster in nature from appearing in a perfect shape.

There are two major types of methods for discovering biclusters in data that may come with noise. **Optimization-based methods** conduct an iterative search. At each iteration, the submatrix with the highest significance score is identified as a bicluster. The process terminates when a user-specified condition is met. Due to cost concerns in computation, greedy search is often employed to find local optimal biclusters. **Enumeration methods** use a tolerance threshold to specify the degree of noise allowed in the biclusters to be mined, and then tries to enumerate all submatrices of biclusters that satisfy the requirements. We use the δ-Cluster and MaPle algorithms as examples to illustrate these ideas.

Optimization Using the δ-Cluster Algorithm

For a submatrix, $I \times J$, the mean of the ith row is

$$e_{iJ} = \frac{1}{|J|} \sum_{j \in J} e_{ij}. \tag{11.16}$$

Symmetrically, the mean of the jth column is

$$e_{Ij} = \frac{1}{|I|} \sum_{i \in I} e_{ij}. \tag{11.17}$$

The mean of all elements in the submatrix is

$$e_{IJ} = \frac{1}{|I||J|} \sum_{i \in I, j \in J} e_{ij} = \frac{1}{|I|} \sum_{i \in I} e_{iJ} = \frac{1}{|J|} \sum_{j \in J} e_{Ij}. \tag{11.18}$$

The quality of the submatrix as a bicluster can be measured by the *mean-squared residue* value as

$$H(I \times J) = \frac{1}{|I||J|} \sum_{i \in I, j \in J} (e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2. \tag{11.19}$$

Submatrix $I \times J$ is a δ-**bicluster** if $H(I \times J) \leq \delta$, where $\delta \geq 0$ is a threshold. When $\delta = 0$, $I \times J$ is a perfect bicluster with coherent values. By setting $\delta > 0$, a user can specify the tolerance of average noise per element against a perfect bicluster, because in Eq. (11.19) the residue on each element is

$$\text{residue}(e_{ij}) = e_{ij} - e_{iJ} - e_{Ij} + e_{IJ}. \tag{11.20}$$

A *maximal* δ*-bicluster* is a δ-bicluster $I \times J$ such that there does not exist another δ-bicluster $I' \times J'$, and $I \subseteq I'$, $J \subseteq J'$, and at least one inequality holds. Finding the maximal δ-bicluster of the largest size is computationally costly. Therefore, we can use a heuristic greedy search method to obtain a local optimal cluster. The algorithm works in two phases.

- In the *deletion phase*, we start from the whole matrix. While the mean-squared residue of the matrix is over δ, we iteratively remove rows and columns. At each iteration, for each row i, we compute the *mean-squared residue* as

$$d(i) = \frac{1}{|J|}\sum_{j\in J}(e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2. \tag{11.21}$$

  Moreover, for each column j, we compute the *mean-squared residue* as

$$d(j) = \frac{1}{|I|}\sum_{i\in I}(e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2. \tag{11.22}$$

  We remove the row or column of the largest mean-squared residue. At the end of this phase, we obtain a submatrix $I \times J$ that is a δ-bicluster. However, the submatrix may not be maximal.

- In the *addition phase*, we iteratively expand the δ-bicluster $I \times J$ obtained in the deletion phase as long as the δ-bicluster requirement is maintained. At each iteration, we consider rows and columns that are not involved in the current bicluster $I \times J$ by calculating their mean-squared residues. A row or column of the smallest mean-squared residue is added into the current δ-bicluster.

This greedy algorithm can find one δ-bicluster only. To find multiple biclusters that do not have heavy overlaps, we can run the algorithm multiple times. After each execution where a δ-bicluster is output, we can replace the elements in the output bicluster by random numbers. Although the greedy algorithm may find neither the optimal biclusters nor all biclusters, it is very fast even on large matrices.

Enumerating All Biclusters Using MaPle

As mentioned, a submatrix $I \times J$ is a bicluster with coherent values if and only if for any $i_1, i_2 \in I$ and $j_1, j_2 \in J$, $e_{i_1 j_1} - e_{i_2 j_1} = e_{i_1 j_2} - e_{i_2 j_2}$. For any 2×2 submatrix of $I \times J$, we can define a *p-score* as

$$p\text{-score}\begin{pmatrix} e_{i_1 j_1} & e_{i_1 j_2} \\ e_{i_2 j_1} & e_{i_2 j_2} \end{pmatrix} = |(e_{i_1 j_1} - e_{i_2 j_1}) - (e_{i_1 j_2} - e_{i_2 j_2})|. \tag{11.23}$$

A submatrix $I \times J$ is a **δ-pCluster** (for *p*attern-based *cluster*) if the p-score of every 2×2 submatrix of $I \times J$ is at most δ, where $\delta \geq 0$ is a threshold specifying a user's tolerance of noise against a perfect bicluster. Here, the p-score controls the noise on every element in a bicluster, while the mean-squared residue captures the average noise.

An interesting property of δ-pCluster is that if $I \times J$ is a δ-pCluster, then every $x \times y$ $(x, y \geq 2)$ submatrix of $I \times J$ is also a δ-pCluster. This monotonicity enables us to obtain a succinct representation of nonredundant δ-pClusters. A δ-pCluster is maximal if no more rows or columns can be added into the cluster while maintaining the δ-pCluster property. To avoid redundancy, instead of finding all δ-pClusters, we only need to compute all maximal δ-pClusters.

MaPle is an algorithm that enumerates all maximal δ-pClusters. It systematically enumerates every combination of conditions using a set enumeration tree and a depth-first search. This enumeration framework is the same as the pattern-growth methods for frequent pattern mining (Chapter 6). Consider gene expression data. For each condition combination, J, MaPle finds the maximal subsets of genes, I, such that $I \times J$ is a δ-pCluster. If $I \times J$ is not a submatrix of another δ-pCluster, then $I \times J$ is a maximal δ-pCluster.

There may be a huge number of condition combinations. MaPle prunes many unfruitful combinations using the monotonicity of δ-pClusters. For a condition combination, J, if there does not exist a set of genes, I, such that $I \times J$ is a δ-pCluster, then we do not need to consider any superset of J. Moreover, we should consider $I \times J$ as a candidate of a δ-pCluster only if for every $(|J| - 1)$-subset J' of J, $I \times J'$ is a δ-pCluster. MaPle also employs several pruning techniques to speed up the search while retaining the completeness of returning all maximal δ-pClusters. For example, when examining a current δ-pCluster, $I \times J$, MaPle collects all the genes and conditions that may be added to expand the cluster. If these candidate genes and conditions together with I and J form a submatrix of a δ-pCluster that has already been found, then the search of $I \times J$ and any superset of J can be pruned. Interested readers may refer to the bibliographic notes for additional information on the MaPle algorithm (Section 11.7).

An interesting observation here is that the search for maximal δ-pClusters in MaPle is somewhat similar to mining frequent closed itemsets. Consequently, MaPle borrows the depth-first search framework and ideas from the pruning techniques of pattern-growth methods for frequent pattern mining. This is an example where frequent pattern mining and cluster analysis may share similar techniques and ideas.

An advantage of MaPle and the other algorithms that enumerate all biclusters is that they guarantee the completeness of the results and do not miss any overlapping biclusters. However, a challenge for such enumeration algorithms is that they may become very time consuming if a matrix becomes very large, such as a customer-purchase matrix of hundreds of thousands of customers and millions of products.

11.2.4 Dimensionality Reduction Methods and Spectral Clustering

Subspace clustering methods try to find clusters in subspaces of the original data space. In some situations, it is more effective to construct a new space instead of using subspaces of the original data. This is the motivation behind dimensionality reduction methods for clustering high-dimensional data.

Example 11.14 **Clustering in a derived space.** Consider the three clusters of points in Figure 11.9. It is not possible to cluster these points in any subspace of the original space, $X \times Y$, because

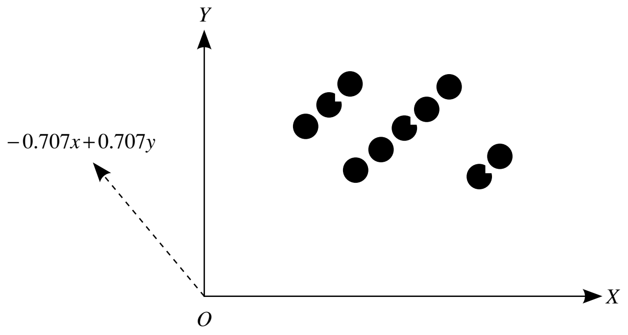


Figure 11.9 Clustering in a derived space may be more effective.

all three clusters would end up being projected onto overlapping areas in the x and y axes. What if, instead, we construct a new dimension, $-\frac{\sqrt{2}}{2}x + \frac{\sqrt{2}}{2}y$ (shown as a dashed line in the figure)? By projecting the points onto this new dimension, the three clusters become apparent. ■

Although Example 11.14 involves only two dimensions, the idea of constructing a new space (so that any clustering structure that is hidden in the data becomes well manifested) can be extended to high-dimensional data. Preferably, the newly constructed space should have low dimensionality.

There are many dimensionality reduction methods. A straightforward approach is to apply feature selection and extraction methods to the data set such as those discussed in Chapter 3. However, such methods may not be able to detect the clustering structure. Therefore, methods that combine feature extraction and clustering are preferred. In this section, we introduce *spectral clustering*, a group of methods that are effective in high-dimensional data applications.

Figure 11.10 shows the general framework for spectral clustering approaches. The Ng-Jordan-Weiss algorithm is a spectral clustering method. Let's have a look at each step of the framework. In doing so, we also note special conditions that apply to the Ng-Jordan-Weiss algorithm as an example.

Given a set of objects, $o_1, \ldots, o_n$, the distance between each pair of objects, $dist(o_i, o_j)$ $(1 \leq i, j \leq n)$, and the desired number k of clusters, a spectral clustering approach works as follows.

1. Using the distance measure, calculate an *affinity matrix*, W, such that

$$W_{ij} = e^{-\frac{dist(o_i,o_j)}{\sigma^2}},$$

where σ is a scaling parameter that controls how fast the affinity W_{ij} decreases as $dist(o_i, o_j)$ increases. In the Ng-Jordan-Weiss algorithm, W_{ii} is set to 0.

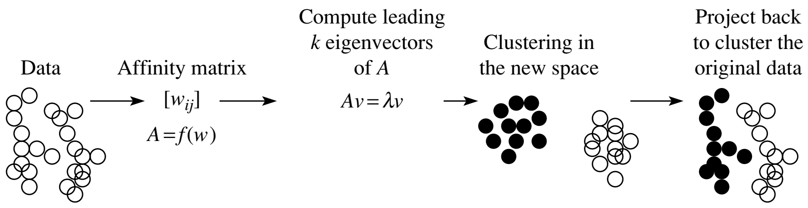

Data
Affinity matrix
$[w_{ij}]$
$A=f(w)$
Compute leading k eigenvectors of A
$Av=\lambda v$
Clustering in the new space
Project back to cluster the original data

Figure 11.10 The framework of spectral clustering approaches. *Source:* Adapted from Slide 8 at *http://videolectures.net/micued08_azran_mcl/*.

2. Using the affinity matrix W, derive a matrix $A = f(W)$. The way in which this is done can vary. The Ng-Jordan-Weiss algorithm defines a matrix, D, as a diagonal matrix such that D_{ii} is the sum of the ith row of W, that is,

$$D_{ii} = \sum_{j=1}^{n} W_{ij}. \tag{11.24}$$

A is then set to

$$A = D^{-\frac{1}{2}} W D^{-\frac{1}{2}}. \tag{11.25}$$

3. Find the k leading eigenvectors of A. Recall that the *eigenvectors* of a square matrix are the nonzero vectors that remain proportional to the original vector after being multiplied by the matrix. Mathematically, a vector $\boldsymbol{v}$ is an eigenvector of matrix A if $A\boldsymbol{v} = \lambda\boldsymbol{v}$, where λ is called the corresponding *eigenvalue*. This step derives k new dimensions from A, which are based on the affinity matrix W. Typically, k should be much smaller than the dimensionality of the original data.

   The Ng-Jordan-Weiss algorithm computes the k eigenvectors with the largest eigenvalues $x_1, \ldots, x_k$ of A.

4. Using the k leading eigenvectors, project the original data into the new space defined by the k leading eigenvectors, and run a clustering algorithm such as k-means to find k clusters.

   The Ng-Jordan-Weiss algorithm stacks the k largest eigenvectors in columns to form a matrix $X = [x_1 x_2 \cdots x_k] \in \mathbb{R}^{n\times k}$. The algorithm forms a matrix Y by renormalizing each row in X to have unit length, that is,

$$Y_{ij} = \frac{X_{ij}}{\sqrt{\sum_{j=1}^{k} X_{ij}^2}}. \tag{11.26}$$

The algorithm then treats each row in Y as a point in the k-dimensional space $\mathbb{R}^k$, and runs k-means (or any other algorithm serving the partitioning purpose) to cluster the points into k clusters.

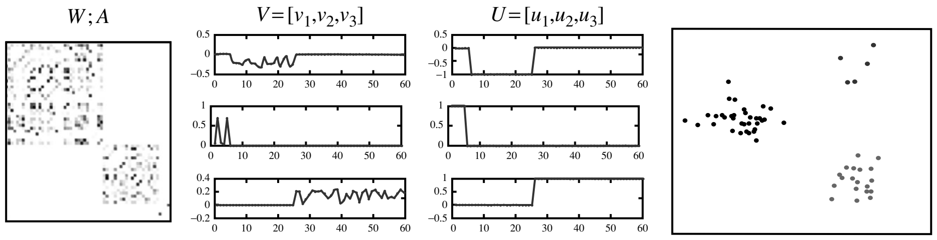


Figure 11.11 The new dimensions and the clustering results of the Ng-Jordan-Weiss algorithm. *Source:* Adapted from Slide 9 at *http://videolectures.net/micued08_azran_mcl/*.

5. Assign the original data points to clusters according to how the transformed points are assigned in the clusters obtained in step 4.

In the Ng-Jordan-Weiss algorithm, the original object o_i is assigned to the jth cluster if and only if matrix Y's row i is assigned to the jth cluster as a result of step 4.

In spectral clustering methods, the dimensionality of the new space is set to the desired number of clusters. This setting expects that each new dimension should be able to manifest a cluster.

Example 11.15 **The Ng-Jordan-Weiss algorithm.** Consider the set of points in Figure 11.11. The data set, the affinity matrix, the three largest eigenvectors, and the normalized vectors are shown. Note that with the three new dimensions (formed by the three largest eigenvectors), the clusters are easily detected. ■

Spectral clustering is effective in high-dimensional applications such as image processing. Theoretically, it works well when certain conditions apply. Scalability, however, is a challenge. Computing eigenvectors on a large matrix is costly. Spectral clustering can be combined with other clustering methods, such as biclustering. Additional information on other dimensionality reduction clustering methods, such as kernel PCA, can be found in the bibliographic notes (Section 11.7).

11.3 Clustering Graph and Network Data

Cluster analysis on graph and network data extracts valuable knowledge and information. Such data are increasingly popular in many applications. We discuss applications and challenges of clustering graph and network data in Section 11.3.1. Similarity measures for this form of clustering are given in Section 11.3.2. You will learn about graph clustering methods in Section 11.3.3.

In general, the terms *graph* and *network* can be used interchangeably. In the rest of this section, we mainly use the term *graph.*

11.3.1 Applications and Challenges

As a customer relationship manager at *AllElectronics*, you notice that a lot of data relating to customers and their purchase behavior can be preferably modeled using graphs.

Example 11.16 **Bipartite graph.** The customer purchase behavior at *AllElectronics* can be represented in a *bipartite graph*. In a bipartite graph, vertices can be divided into two disjoint sets so that each edge connects a vertex in one set to a vertex in the other set. For the *AllElectronics* customer purchase data, one set of vertices represents customers, with one customer per vertex. The other set represents products, with one product per vertex. An edge connects a customer to a product, representing the purchase of the product by the customer. Figure 11.12 shows an illustration.

"*What kind of knowledge can we obtain by a cluster analysis of the customer-product bipartite graph?*" By clustering the customers such that those customers buying similar sets of products are placed into one group, a customer relationship manager can make product recommendations. For example, suppose Ada belongs to a customer cluster in which most of the customers purchased a digital camera in the last 12 months, but Ada has yet to purchase one. As manager, you decide to recommend a digital camera to her.

Alternatively, we can cluster products such that those products purchased by similar sets of customers are grouped together. This clustering information can also be used for product recommendations. For example, if a digital camera and a high-speed flash memory card belong to the same product cluster, then when a customer purchases a digital camera, we can recommend the high-speed flash memory card. ■

Bipartite graphs are widely used in many applications. Consider another example.

Example 11.17 **Web search engines.** In web search engines, search logs are archived to record user queries and the corresponding *click-through information*. (The click-through information tells us on which pages, given as a result of a search, the user clicked.) The query and click-through information can be represented using a bipartite graph, where the two sets

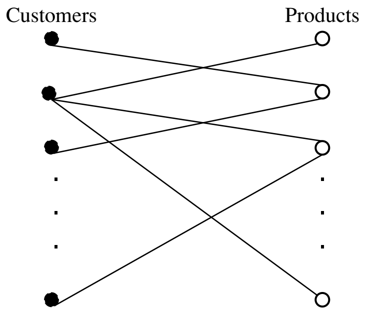


Figure 11.12 Bipartite graph representing customer-purchase data.

of vertices correspond to queries and web pages, respectively. An edge links a query to a web page if a user clicks the web page when asking the query. Valuable information can be obtained by cluster analyses on the query–web page bipartite graph. For instance, we may identify queries posed in different languages, but that mean the same thing, if the click-through information for each query is similar.

As another example, all the web pages on the Web form a directed graph, also known as the *web graph*, where each web page is a vertex, and each hyperlink is an edge pointing from a source page to a destination page. Cluster analysis on the web graph can disclose communities, find hubs and authoritative web pages, and detect web spams. ■

In addition to bipartite graphs, cluster analysis can also be applied to other types of graphs, including general graphs, as elaborated Example 11.18.

Example 11.18 **Social network.** A *social network* is a social structure. It can be represented as a graph, where the vertices are individuals or organizations, and the links are interdependencies between the vertices, representing friendship, common interests, or collaborative activities. *AllElectronics*' customers form a social network, where each customer is a vertex, and an edge links two customers if they know each other.

As customer relationship manager, you are interested in finding useful information that can be derived from *AllElectronics*' social network through cluster analysis. You obtain clusters from the network, where customers in a cluster know each other or have friends in common. Customers within a cluster may influence one another regarding purchase decision making. Moreover, communication channels can be designed to inform the "heads" of clusters (i.e., the "best" connected people in the clusters), so that promotional information can be spread out quickly. Thus, you may use customer clustering to promote sales at *AllElectronics*.

As another example, the authors of scientific publications form a social network, where the authors are vertices and two authors are connected by an edge if they coauthored a publication. The network is, in general, a weighted graph because an edge between two authors can carry a weight representing the strength of the collaboration such as how many publications the two authors (as the end vertices) coauthored. Clustering the coauthor network provides insight as to communities of authors and patterns of collaboration. ■

"Are there any challenges specific to cluster analysis on graph and network data?" In most of the clustering methods discussed so far, objects are represented using a set of attributes. A unique feature of graph and network data is that only objects (as vertices) and relationships between them (as edges) are given. No dimensions or attributes are explicitly defined. To conduct cluster analysis on graph and network data, there are two major new challenges.

- *"How can we measure the similarity between two objects on a graph accordingly?"* Typically, we cannot use conventional distance measures, such as Euclidean distance. Instead, we need to develop new measures to quantify the similarity. Such measures often are not metric, and thus raise new challenges regarding the development of efficient clustering methods. Similarity measures for graphs are discussed in Section 11.3.2.

- *"How can we design clustering models and methods that are effective on graph and network data?"* Graph and network data are often complicated, carrying topological structures that are more sophisticated than traditional cluster analysis applications. Many graph data sets are large, such as the web graph containing at least tens of billions of web pages in the publicly indexable Web. Graphs can also be sparse where, on average, a vertex is connected to only a small number of other vertices in the graph. To discover accurate and useful knowledge hidden deep in the data, a good clustering method has to accommodate these factors. Clustering methods for graph and network data are introduced in Section 11.3.3.

11.3.2 Similarity Measures

"How can we measure the similarity or distance between two vertices in a graph?" In our discussion, we examine two types of measures: *geodesic distance* and *distance based on random walk.*

Geodesic Distance

A simple measure of the distance between two vertices in a graph is the shortest path between the vertices. Formally, the **geodesic distance** between two vertices is the length in terms of the number of edges of the shortest path between the vertices. For two vertices that are not connected in a graph, the geodesic distance is defined as infinite.

Using geodesic distance, we can define several other useful measurements for graph analysis and clustering. Given a graph $G = (V, E)$, where V is the set of vertices and E is the set of edges, we define the following:

- For a vertext $v \in V$, the **eccentricity** of v, denoted $eccen(v)$, is the largest geodesic distance between v and any other vertex $u \in V - \{v\}$. The eccentricity of v captures how far away v is from its remotest vertex in the graph.
- The **radius** of graph G is the minimum eccentricity of all vertices. That is,

$$r = \min_{v \in V} eccen(v). \tag{11.27}$$

  The radius captures the distance between the "most central point" and the "farthest border" of the graph.
- The **diameter** of graph G is the maximum eccentricity of all vertices. That is,

$$d = \max_{v \in V} eccen(v). \tag{11.28}$$

  The diameter represents the largest distance between any pair of vertices.
- A **peripheral vertex** is a vertex that achieves the diameter.

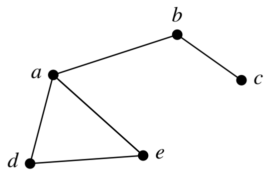


Figure 11.13 A graph, G, where vertices c, d, and e are peripheral.

Example 11.19 **Measurements based on geodesic distance.** Consider graph G in Figure 11.13. The eccentricity of a is 2, that is, $eccen(a) = 2$, $eccen(b) = 2$, and $eccen(c) = eccen(d) = eccen(e) = 3$. Thus, the radius of G is 2, and the diameter is 3. Note that it is not necessary that $d = 2 \times r$. Vertices c, d, and e are peripheral vertices. ■

SimRank: Similarity Based on Random Walk and Structural Context

For some applications, geodesic distance may be inappropriate in measuring the similarity between vertices in a graph. Here we introduce SimRank, a similarity measure based on random walk and on the structural context of the graph. In mathematics, a *random walk* is a trajectory that consists of taking successive random steps.

Example 11.20 **Similarity between people in a social network.** Let's consider measuring the similarity between two vertices in the *AllElectronics* customer social network of Example 11.18. Here, similarity can be explained as the closeness between two participants in the network, that is, how close two people are in terms of the relationship represented by the social network.

"*How well can the geodesic distance measure similarity and closeness in such a network?*" Suppose Ada and Bob are two customers in the network, and the network is undirected. The geodesic distance (i.e., the length of the shortest path between Ada and Bob) is the shortest path that a message can be passed from Ada to Bob and vice versa. However, this information is not useful for *AllElectronics*' customer relationship management because the company typically does not want to send a specific message from one customer to another. Therefore, geodesic distance does not suit the application.

"*What does similarity mean in a social network?*" We consider two ways to define similarity:

- Two customers are considered similar to one another if they have similar neighbors in the social network. This heuristic is intuitive because, in practice, two people receiving recommendations from a good number of common friends often make similar decisions. This kind of similarity is based on the local structure (i.e., the *neighborhoods*) of the vertices, and thus is called *structural context–based similarity*.

- Suppose *AllElectronics* sends promotional information to both Ada and Bob in the social network. Ada and Bob may randomly forward such information to their friends (or *neighbors*) in the network. The closeness between Ada and Bob can then be measured by the likelihood that other customers simultaneously receive the promotional information that was originally sent to Ada and Bob. This kind of similarity is based on the random walk reachability over the network, and thus is referred to as *similarity based on random walk.* ■

Let's have a closer look at what is meant by similarity based on structural context, and similarity based on random walk.

The intuition behind similarity based on structural context is that two vertices in a graph are similar if they are connected to similar vertices. To measure such similarity, we need to define the notion of individual neighborhood. In a directed graph $G = (V, E)$, where V is the set of vertices and $E \subseteq V \times V$ is the set of edges, for a vertex $v \in V$, the *individual in-neighborhood* of v is defined as

$$I(v) = \{u | (u, v) \in E\}. \tag{11.29}$$

Symmetrically, we define the *individual out-neighborhood* of v as

$$O(v) = \{w | (v, w) \in E\}. \tag{11.30}$$

Following the intuition illustrated in Example 11.20, we define SimRank, a structural-context similarity, with a value that is between 0 and 1 for any pair of vertices. For any vertex, $v \in V$, the similarity between the vertex and itself is $s(v, v) = 1$ because the neighborhoods are identical. For vertices $u, v \in V$ such that $u \neq v$, we can define

$$s(u, v) = \frac{C}{|I(u)||I(v)|} \sum_{x \in I(u)} \sum_{y \in I(v)} s(x, y), \tag{11.31}$$

where C is a constant between 0 and 1. A vertex may not have any in-neighbors. Thus, we define Eq. (11.31) to be 0 when either $I(u)$ or $I(v)$ is $\emptyset$. Parameter C specifies the rate of decay as similarity is propagated across edges.

"How can we compute SimRank?" A straightforward method iteratively evaluates Eq. (11.31) until a fixed point is reached. Let $s_i(u, v)$ be the SimRank score calculated at the ith round. To begin, we set

$$s_0(u, v) = \begin{cases} 0 & \text{if } u \neq v \\ 1 & \text{if } u = v. \end{cases} \tag{11.32}$$

We use Eq. (11.31) to compute s_{i+1} from s_i as

$$s_{i+1}(u, v) = \frac{C}{|I(u)||I(v)|} \sum_{x \in I(u)} \sum_{y \in I(v)} s_i(x, y). \tag{11.33}$$

It can be shown that $\lim_{i\to\infty} s_i(u,v) = s(u,v)$. Additional methods for approximating SimRank are given in the bibliographic notes (Section 11.7).

Now, let's consider similarity based on random walk. A directed graph is *strongly connected* if, for any two nodes u and v, there is a path from u to v and another path from v to u. In a strongly connected graph, $G = (V,E)$, for any two vertices, $u, v \in V$, we can define the *expected distance* from u to v as

$$d(u,v) = \sum_{t:u \rightsquigarrow v} P[t]l(t), \tag{11.34}$$

where $u \rightsquigarrow v$ is a path starting from u and ending at v that may contain cycles but does not reach v until the end. For a *traveling tour*, $t = w_1 \to w_2 \to \cdots \to w_k$, its length is $l(t) = k-1$. The probability of the tour is defined as

$$P[t] = \begin{cases} \prod_{i=1}^{k-1} \frac{1}{|O(w_i)|} & \text{if } l(t) > 0 \\ 0 & \text{if } l(t) = 0. \end{cases} \tag{11.35}$$

To measure the probability that a vertex w receives a message that originated simultaneously from u and v, we extend the expected distance to the notion of *expected meeting distance*, that is,

$$m(u,v) = \sum_{t:(u,v) \rightsquigarrow (x,x)} P[t]l(t), \tag{11.36}$$

where $(u,v) \rightsquigarrow (x,x)$ is a pair of tours $u \rightsquigarrow x$ and $v \rightsquigarrow x$ of the same length. Using a constant C between 0 and 1, we define the *expected meeting probability* as

$$p(u,v) = \sum_{t:(u,v) \rightsquigarrow (x,x)} P[t]C^{l(t)}, \tag{11.37}$$

which is a similarity measure based on random walk. Here, the parameter C specifies the probability of continuing the walk at each step of the trajectory.

It has been shown that $s(u,v) = p(u,v)$ for any two vertices, u and v. That is, SimRank is based on both structural context and random walk.

11.3.3 Graph Clustering Methods

Let's consider how to conduct clustering on a graph. We first describe the intuition behind graph clustering. We then discuss two general categories of graph clustering methods.

To find clusters in a graph, imagine cutting the graph into pieces, each piece being a cluster, such that the vertices within a cluster are well connected and the vertices in different clusters are connected in a much weaker way. Formally, for a graph, $G = (V,E)$, a **cut**, $C = (S, T)$, is a partitioning of the set of vertices V in G, that is, $V = S \cup T$ and $S \cap T = \emptyset$. The *cut set* of a cut is the set of edges, $\{(u, v) \in E | u \in S, v \in T\}$. The *size* of the cut is the number of edges in the cut set. For weighted graphs, the size of a cut is the sum of the weights of the edges in the cut set.

"What kinds of cuts are good for deriving clusters in graphs?" In graph theory and some network applications, a minimum cut is of importance. A cut is *minimum* if the cut's size is not greater than any other cut's size. There are polynomial time algorithms to compute minimum cuts of graphs. Can we use these algorithms in graph clustering?

Example 11.21 **Cuts and clusters.** Consider graph G in Figure 11.14. The graph has two clusters: $\{a, b, c, d, e, f\}$ and $\{g, h, i, j, k\}$, and one outlier vertex, l.

Consider cut $C_1 = (\{a, b, c, d, e, f, g, h, i, j, k\}, \{l\})$. Only one edge, namely, (e, l), crosses the two partitions created by C_1. Therefore, the cut set of C_1 is $\{(e, l)\}$ and the size of C_1 is 1. (Note that the size of any cut in a connected graph cannot be smaller than 1.) As a minimum cut, C_1 does not lead to a good clustering because it only separates the outlier vertex, l, from the rest of the graph.

Cut $C_2 = (\{a, b, c, d, e, f, l\}, \{g, h, i, j, k\})$ leads to a much better clustering than C_1. The edges in the cut set of C_2 are those connecting the two "natural clusters" in the graph. Specifically, for edges (d, h) and (e, k) that are in the cut set, most of the edges connecting d, h, e, and k belong to one cluster. ■

Example 11.21 indicates that using a minimum cut is unlikely to lead to a good clustering. We are better off choosing a cut where, for each vertex u that is involved in an edge in the cut set, most of the edges connecting to u belong to one cluster. Formally, let $deg(u)$ be the degree of u, that is, the number of edges connecting to u. The *sparsity* of a cut $C = (S, T)$ is defined as

$$\Phi = \frac{\text{cut size}}{\min\{|S|, |T|\}}. \tag{11.38}$$

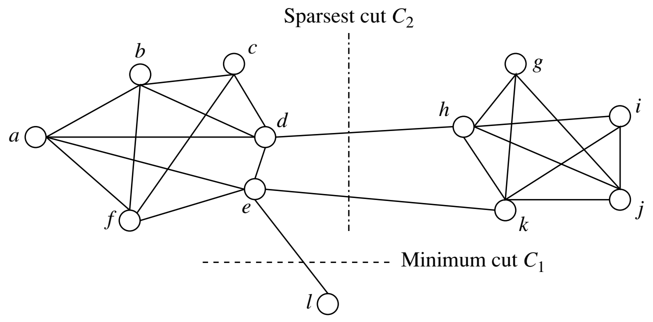


Figure 11.14 A graph G and two cuts.

A cut is *sparsest* if its sparsity is not greater than the sparsity of any other cut. There may be more than one sparsest cut.

In Example 11.21 and Figure 11.14, C_2 is a sparsest cut. Using sparsity as the objective function, a sparsest cut tries to minimize the number of edges crossing the partitions and balance the partitions in size.

Consider a clustering on a graph $G = (V, E)$ that partitions the graph into k clusters. The **modularity** of a clustering assesses the quality of the clustering and is defined as

$$Q = \sum_{i=1}^{k} \left(\frac{l_i}{|E|} - \left(\frac{d_i}{2|E|} \right)^2 \right), \tag{11.39}$$

where l_i is the number of edges between vertices in the ith cluster, and d_i is the sum of the degrees of the vertices in the ith cluster. The modularity of a clustering of a graph is the difference between the fraction of all edges that fall into individual clusters and the fraction that would do so if the graph vertices were randomly connected. The optimal clustering of graphs maximizes the modularity.

Theoretically, many graph clustering problems can be regarded as finding good cuts, such as the sparsest cuts, on the graph. In practice, however, a number of challenges exist:

- **High computational cost:** Many graph cut problems are computationally expensive. The sparsest cut problem, for example, is NP-hard. Therefore, finding the optimal solutions on large graphs is often impossible. A good trade-off between efficiency/scalability and quality has to be achieved.
- **Sophisticated graphs:** Graphs can be more sophisticated than the ones described here, involving weights and/or cycles.
- **High dimensionality:** A graph can have many vertices. In a similarity matrix, a vertex is represented as a vector (a row in the matrix) with a dimensionality that is the number of vertices in the graph. Therefore, graph clustering methods must handle high dimensionality.
- **Sparsity:** A large graph is often sparse, meaning each vertex on average connects to only a small number of other vertices. A similarity matrix from a large sparse graph can also be sparse.

There are two kinds of methods for clustering graph data, which address these challenges. One uses clustering methods for high-dimensional data, while the other is designed specifically for clustering graphs.

The first group of methods is based on generic clustering methods for high-dimensional data. They extract a similarity matrix from a graph using a similarity measure such as those discussed in Section 11.3.2. A generic clustering method can then be applied on the similarity matrix to discover clusters. Clustering methods for high-dimensional data are typically employed. For example, in many scenarios, once a similarity matrix is obtained, spectral clustering methods (Section 11.2.4) can be applied. Spectral clustering can approximate optimal graph cut solutions. For additional information, please refer to the bibliographic notes (Section 11.7).

The second group of methods is specific to graphs. They search the graph to find well-connected components as clusters. Let's look at a method called **SCAN** (Structural Clustering Algorithm for Networks) as an example.

Given an undirected graph, $G = (V, E)$, for a vertex, $u \in V$, the neighborhood of u is $\Gamma(u) = \{v | (u, v) \in E\} \cup \{u\}$. Using the idea of structural-context similarity, SCAN measures the similarity between two vertices, $u, v \in V$, by the normalized common neighborhood size, that is,

$$\sigma(u, v) = \frac{|\Gamma(u) \cap \Gamma(v)|}{\sqrt{|\Gamma(u)||\Gamma(v)|}}. \tag{11.40}$$

The larger the value computed, the more similar the two vertices. SCAN uses a similarity threshold ε to define the cluster membership. For a vertex, $u \in V$, the *ε-neighborhood* of u is defined as $N_\varepsilon(u) = \{v \in \Gamma(u) | \sigma(u, v) \geq \varepsilon\}$. The ε-neighborhood of u contains all neighbors of u with a structural-context similarity to u that is at least ε.

In SCAN, a *core vertex* is a vertex inside of a cluster. That is, $u \in V$ is a core vertex if $|N_\varepsilon(u)| \geq \mu$, where μ is a popularity threshold. SCAN grows clusters from core vertices. If a vertex v is in the ε-neighborhood of a core u, then v is assigned to the same cluster as u. This process of growing clusters continues until no cluster can be further grown. The process is similar to the density-based clustering method, DBSCAN (Chapter 10).

Formally, a vertex v can be *directly reached* from a core u if $v \in N_\varepsilon(u)$. Transitively, a vertex v can be *reached* from a core u if there exist vertices $w_1, \ldots, w_n$ such that w_1 can be reached from u, w_i can be reached from w_{i-1} for $1 < i \leq n$, and v can be reached from w_n. Moreover, two vertices, $u, v \in V$, which may or may not be cores, are said to be *connected* if there exists a core w such that both u and v can be reached from w. All vertices in a cluster are connected. A cluster is a maximum set of vertices such that every pair in the set is connected.

Some vertices may not belong to any cluster. Such a vertex u is a *hub* if the neighborhood $\Gamma(u)$ of u contains vertices from more than one cluster. If a vertex does not belong to any cluster, and is not a hub, it is an *outlier*.

The SCAN algorithm is shown in Figure 11.15. The search framework closely resembles the cluster-finding process in DBSCAN. SCAN finds a cut of the graph, where each cluster is a set of vertices that are connected based on the transitive similarity in a structural context.

An advantage of SCAN is that its time complexity is linear with respect to the number of edges. In very large and sparse graphs, the number of edges is in the same scale of the number of vertices. Therefore, SCAN is expected to have good scalability on clustering large graphs.

```
Algorithm: SCAN for clusters on graph data.
Input: a graph $G = (V, E)$, a similarity threshold $\varepsilon$, and a
   population threshold $\mu$
Output: a set of clusters
Method: set all vertices in $V$ unlabeled
   for all unlabeled vertex $u$ do
      if $u$ is a core then
         generate a new cluster-id $c$
         insert all $v \in N_\varepsilon(u)$ into a queue $Q$
         while $Q \neq$ do
            $w \leftarrow$ the first vertex in $Q$
            $R \leftarrow$ the set of vertices that can be directly reached from $w$
            for all $s \in R$ do
               if $s$ is not unlabeled or labeled as nonmember then
                  assign the current cluster-id $c$ to $s$
               endif
               if $s$ is unlabeled then
                  insert $s$ into queue $Q$
               endif
            endfor
            remove $w$ from $Q$
         end while
      else
         label $u$ as nonmember
      endif
   endfor
   for all vertex $u$ labeled nonmember do
      if $\exists x, y \in \Gamma(u)$ : $x$ and $y$ have different cluster-ids then
         label $u$ as hub
      else
         label $u$ as outlier
      endif
   endfor
```

Figure 11.15 SCAN algorithm for cluster analysis on graph data.

11.4 Clustering with Constraints

Users often have background knowledge that they want to integrate into cluster analysis. There may also be application-specific requirements. Such information can be modeled as clustering constraints. We approach the topic of clustering with constraints in two steps. Section 11.4.1 categorizes the types of constraints for clustering graph data. Methods for clustering with constraints are introduced in Section 11.4.2.

11.4.1 Categorization of Constraints

This section studies how to categorize the constraints used in cluster analysis. Specifically, we can categorize constraints according to the subjects on which they are set, or on how strongly the constraints are to be enforced.

As discussed in Chapter 10, cluster analysis involves three essential aspects: objects as instances of clusters, clusters as groups of objects, and the similarity among objects. Therefore, the first method we discuss categorizes constraints according to what they are applied to. We thus have three types: *constraints on instances*, *constraints on clusters*, and *constraints on similarity measurement.*

Constraints on instances: A *constraint on instances* specifies how a pair or a set of instances should be grouped in the cluster analysis. Two common types of constraints from this category include:

- **Must-link constraints.** If a must-link constraint is specified on two objects x and y, then x and y should be grouped into one cluster in the output of the cluster analysis. These must-link constraints are transitive. That is, if must-link(x, y) and must-link(y, z), then must-link(x, z).
- **Cannot-link constraints.** Cannot-link constraints are the opposite of must-link constraints. If a cannot-link constraint is specified on two objects, x and y, then in the output of the cluster analysis, x and y should belong to different clusters. Cannot-link constraints can be entailed. That is, if cannot-link(x, y), must-link(x, x'), and must-link(y, y'), then cannot-link(x', y').

A constraint on instances can be defined using specific instances. Alternatively, it can also be defined using instance variables or attributes of instances. For example, a constraint,

$$Constraint(x, y) : \text{must-link}(x, y) \text{ if } dist(x, y) \leq \epsilon,$$

uses the distance between objects to specify a must-link constraint.

Constraints on clusters: A *constraint on clusters* specifies a requirement on the clusters, possibly using attributes of the clusters. For example, a constraint may specify the minimum number of objects in a cluster, the maximum diameter of a cluster, or the shape of a cluster (e.g., a convex). The number of clusters specified for partitioning clustering methods can be regarded as a constraint on clusters.

Constraints on similarity measurement: Often, a similarity measure, such as Euclidean distance, is used to measure the similarity between objects in a cluster analysis. In some applications, exceptions apply. A *constraint on similarity measurement* specifies a requirement that the similarity calculation must respect. For example, to cluster people as moving objects in a plaza, while Euclidean distance is used to give the walking distance between two points, a constraint on similarity measurement is that the trajectory implementing the shortest distance cannot cross a wall.

There can be more than one way to express a constraint, depending on the category. For example, we can specify a constraint on clusters as

$$Constraint_1\text{: the diameter of a cluster cannot be larger than } d.$$

The requirement can also be expressed using a constraint on instances as

$$Constraint'_1\text{: cannot-link}(x, y) \text{ if } dist(x, y) > d. \tag{11.41}$$

Example 11.22 **Constraints on instances, clusters, and similarity measurement.** *AllElectronics* clusters its customers so that each group of customers can be assigned to a customer relationship manager. Suppose we want to specify that all customers at the same address are to be placed in the same group, which would allow more comprehensive service to families. This can be expressed using a must-link constraint on instances:

$$Constraint_{family}(x, y) : \text{must-link}(x, y) \text{ if } x.address = y.address.$$

AllElectronics has eight customer relationship managers. To ensure that they each have a similar workload, we place a constraint on clusters such that there should be eight clusters, and each cluster should have at least 10% of the customers and no more than 15% of the customers. We can calculate the spatial distance between two customers using the driving distance between the two. However, if two customers live in different countries, we have to use the flight distance instead. This is a constraint on similarity measurement. ■

Another way to categorize clustering constraints considers how firmly the constraints have to be respected. A constraint is **hard** if a clustering that violates the constraint is unacceptable. A constraint is **soft** if a clustering that violates the constraint is not preferable but acceptable when no better solution can be found. Soft constraints are also called *preferences*.

Example 11.23 **Hard and soft constraints.** For *AllElectronics*, $Constraint_{family}$ in Example 11.22 is a hard constraint because splitting a family into different clusters could prevent the company from providing comprehensive services to the family, leading to poor customer satisfaction. The constraint on the number of clusters (which corresponds to the number of customer relationship managers in the company) is also hard. Example 11.22 also has a constraint to balance the size of clusters. While satisfying this constraint is strongly preferred, the company is flexible in that it is willing to assign a senior and more capable customer relationship manager to oversee a larger cluster. Therefore, the constraint is soft. ■

Ideally, for a specific data set and a set of constraints, all clusterings satisfy the constraints. However, it is possible that there may be no clustering of the data set that satisfies all the constraints. Trivially, if two constraints in the set conflict, then no clustering can satisfy them at the same time.

Example 11.24 Conflicting constraints. Consider these constraints:

$$\text{must-link}(x, y) \text{ if } dist(x, y) < 5$$
$$\text{cannot-link}(x, y) \text{ if } dist(x, y) > 3.$$

If a data set has two objects, x, y, such that $dist(x, y) = 4$, then no clustering can satisfy both constraints simultaneously.

Consider these two constraints:

$$\text{must-link}(x, y) \text{ if } dist(x, y) < 5$$
$$\text{must-link}(x, y) \text{ if } dist(x, y) < 3.$$

The second constraint is redundant given the first. Moreover, for a data set where the distance between any two objects is at least 5, every possible clustering of the objects satisfies the constraints. ■

"How can we measure the quality and the usefulness of a set of constraints?" In general, we consider either their informativeness, or their coherence. The **informativeness** is the amount of information carried by the constraints that is beyond the clustering model. Given a data set, D, a clustering method, $\mathcal{A}$, and a set of constraints, $\mathcal{C}$, the informativeness of $\mathcal{C}$ with respect to $\mathcal{A}$ on D can be measured by the fraction of constraints in $\mathcal{C}$ that are unsatisfied by the clustering computed by $\mathcal{A}$ on D. The higher the informativeness, the more specific the requirements and background knowledge that the constraints carry. The **coherence** of a set of constraints is the degree of agreement among the constraints themselves, which can be measured by the redundancy among the constraints.

11.4.2 Methods for Clustering with Constraints

Although we can categorize clustering constraints, applications may have very different constraints of specific forms. Consequently, various techniques are needed to handle specific constraints. In this section, we discuss the general principles of handling hard and soft constraints.

Handling Hard Constraints

A general strategy for handling hard constraints is to strictly respect the constraints in the cluster assignment process. To illustrate this idea, we will use partitioning clustering as an example.

Given a data set and a set of constraints on instances (i.e., must-link or cannot-link constraints), how can we extend the k-means method to satisfy such constraints? The **COP-k-means algorithm** works as follows:

1. **Generate superinstances for must-link constraints**. Compute the transitive closure of the must-link constraints. Here, all must-link constraints are treated as an equivalence relation. The closure gives one or multiple subsets of objects where all objects in a subset must be assigned to one cluster. To represent such a subset, we replace all those objects in the subset by the mean. The superinstance also carries a weight, which is the number of objects it represents.

   After this step, the must-link constraints are always satisfied.

2. **Conduct modified k-means clustering.** Recall that, in k-means, an object is assigned to the closest center. What if a nearest-center assignment violates a cannot-link constraint? To respect cannot-link constraints, we modify the center assignment process in k-means to a *nearest feasible center assignment*. That is, when the objects are assigned to centers in sequence, at each step we make sure the assignments so far do not violate any cannot-link constraints. An object is assigned to the nearest center so that the assignment respects all cannot-link constraints.

Because COP-k-means ensures that no constraints are violated at every step, it does not require any backtracking. It is a greedy algorithm for generating a clustering that satisfies all constraints, provided that no conflicts exist among the constraints.

Handling Soft Constraints

Clustering with soft constraints is an optimization problem. When a clustering violates a soft constraint, a penalty is imposed on the clustering. Therefore, the optimization goal of the clustering contains two parts: optimizing the clustering quality and minimizing the constraint violation penalty. The overall objective function is a combination of the clustering quality score and the penalty score.

To illustrate, we again use partitioning clustering as an example. Given a data set and a set of soft constraints on instances, the **CVQE** (**Constrained Vector Quantization Error**) **algorithm** conducts k-means clustering while enforcing constraint violation penalties. The objective function used in CVQE is the sum of the distance used in k-means, adjusted by the constraint violation penalties, which are calculated as follows.

- **Penalty of a must-link violation.** If there is a must-link constraint on objects x and y, but they are assigned to two different centers, c_1 and c_2, respectively, then the constraint is violated. As a result, $dist(c_1, c_2)$, the distance between c_1 and c_2, is added to the objective function as the penalty.
- **Penalty of a cannot-link violation.** If there is a cannot-link constraint on objects x and y, but they are assigned to a common center, c, then the constraint is violated.

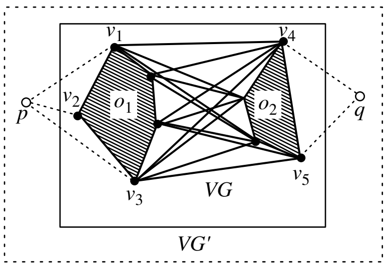
The distance, $dist(c, c')$, between c and c' is added to the objective function as the penalty.

Speeding up Constrained Clustering

Constraints, such as on similarity measurements, can lead to heavy costs in clustering. Consider the following **clustering with obstacles** problem: To cluster people as moving objects in a plaza, Euclidean distance is used to measure the walking distance between two points. However, a constraint on similarity measurement is that the trajectory implementing the shortest distance cannot cross a wall (Section 11.4.1). Because obstacles may occur between objects, the distance between two objects may have to be derived by geometric computations (e.g., involving triangulation). The computational cost is high if a large number of objects and obstacles are involved.

The clustering with obstacles problem can be represented using a graphical notation. First, a point, $\boldsymbol{p}$, is **visible** from another point, $\boldsymbol{q}$, in the region R if the straight line joining $\boldsymbol{p}$ and $\boldsymbol{q}$ does not intersect any obstacles. A **visibility graph** is the graph, $VG = (V, E)$, such that each vertex of the obstacles has a corresponding node in V and two nodes, $\boldsymbol{v_1}$ and $\boldsymbol{v_2}$, in V are joined by an edge in E if and only if the corresponding vertices they represent are visible to each other. Let $VG' = (V', E')$ be a visibility graph created from VG by adding two additional points, $\boldsymbol{p}$ and $\boldsymbol{q}$, in V'. E' contains an edge joining two points in V' if the two points are mutually visible. The shortest path between two points, $\boldsymbol{p}$ and $\boldsymbol{q}$, will be a subpath of VG', as shown in Figure 11.16(a). We see that it begins with an edge from $\boldsymbol{p}$ to either $\boldsymbol{v_1}$, $\boldsymbol{v_2}$, or $\boldsymbol{v_3}$, goes through a path in VG, and then ends with an edge from either $\boldsymbol{v_4}$ or $\boldsymbol{v_5}$ to $\boldsymbol{q}$.

To reduce the cost of distance computation between any two pairs of objects or points, several preprocessing and optimization techniques can be used. One method groups points that are close together into microclusters. This can be done by first triangulating the region R into triangles, and then grouping nearby points in the same triangle into microclusters, using a method similar to BIRCH or DBSCAN, as shown in Figure 11.16(b). By processing microclusters rather than individual points, the overall computation is reduced. After that, precomputation can be performed to build two



(a)

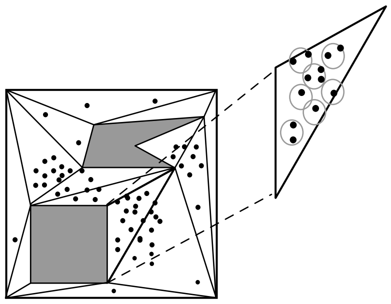

(b)

Figure 11.16 Clustering with obstacle objects (o_1 and o_2): (a) a visibility graph and (b) triangulation of regions with microclusters. *Source:* Adapted from Tung, Hou, and Han [THH01].

kinds of join indices based on the computation of the shortest paths: (1) *VV indices*, for any pair of obstacle vertices, and (2) *MV indices*, for any pair of microcluster and obstacle vertex. Use of the indices helps further optimize the overall performance.

Using such precomputation and optimization strategies, the distance between any two points (at the granularity level of a microcluster) can be computed efficiently. Thus, the clustering process can be performed in a manner similar to a typical efficient *k*-medoids algorithm, such as CLARANS, and achieve good clustering quality for large data sets.

11.5 Summary

- In conventional cluster analysis, an object is assigned to one cluster exclusively. However, in some applications, there is a need to assign an object to one or more clusters in a fuzzy or probabilistic way. **Fuzzy clustering** and **probabilistic model-based clustering** allow an object to belong to one or more clusters. A **partition matrix** records the membership degree of objects belonging to clusters.
- **Probabilistic model-based clustering** assumes that a cluster is a parameterized distribution. Using the data to be clustered as the observed samples, we can estimate the parameters of the clusters.
- A **mixture model** assumes that a set of observed objects is a mixture of instances from multiple probabilistic clusters. Conceptually, each observed object is generated independently by first choosing a probabilistic cluster according to the probabilities of the clusters, and then choosing a sample according to the probability density function of the chosen cluster.
- An **expectation-maximization algorithm** is a framework for approaching maximum likelihood or maximum a posteriori estimates of parameters in statistical models. Expectation-maximization algorithms can be used to compute fuzzy clustering and probabilistic model-based clustering.
- **High-dimensional data** pose several challenges for cluster analysis, including how to model high-dimensional clusters and how to search for such clusters.
- There are two major categories of clustering methods for high-dimensional data: subspace clustering methods and dimensionality reduction methods. **Subspace clustering methods** search for clusters in subspaces of the original space. Examples include **subspace search methods**, **correlation-based clustering methods**, and **biclustering methods**. **Dimensionality reduction methods** create a new space of lower dimensionality and search for clusters there.
- **Biclustering methods** cluster objects and attributes simultaneously. Types of biclusters include biclusters with **constant values**, **constant values on rows/columns**, **coherent values**, and **coherent evolutions on rows/columns**. Two major types of biclustering methods are **optimization-based methods** and **enumeration methods**.

- **Spectral clustering** is a **dimensionality reduction method**. The general idea is to construct new dimensions using an affinity matrix.
- **Clustering graph and network data** has many applications such as social network analysis. Challenges include how to measure the similarity between objects in a graph, and how to design clustering models and methods for graph and network data.
- **Geodesic distance** is the number of edges between two vertices on a graph. It can be used to measure similarity. Alternatively, similarity in graphs, such as social networks, can be measured using structural context and random walk. **SimRank** is a similarity measure that is based on both structural context and random walk.
- Graph clustering can be modeled as computing **graph cuts**. A **sparsest cut** may lead to a good clustering, while **modularity** can be used to measure the clustering quality.
- **SCAN** is a graph clustering algorithm that searches graphs to identify well-connected components as clusters.
- **Constraints** can be used to express application-specific requirements or background knowledge for cluster analysis. Constraints for clustering can be categorized as constraints on **instances**, on **clusters**, or on **similarity measurement**. Constraints on instances include **must-link** and **cannot-link** constraints. A constraint can be **hard** or **soft**.
- **Hard constraints for clustering** can be enforced by strictly respecting the constraints in the cluster assignment process. **Clustering with soft constraints** can be considered an optimization problem. Heuristics can be used to speed up constrained clustering.

11.6 Exercises

11.1 Traditional clustering methods are rigid in that they require each object to belong exclusively to only one cluster. Explain why this is a special case of fuzzy clustering. You may use *k*-means as an example.

11.2 *AllElectronics* carries 1000 products, $P_1, \ldots, P_{1000}$. Consider customers Ada, Bob, and Cathy such that Ada and Bob purchase three products in common, P_1, P_2, and P_3. For the other 997 products, Ada and Bob independently purchase seven of them randomly. Cathy purchases 10 products, randomly selected from the 1000 products. In Euclidean distance, what is the probability that $dist(\text{Ada}, \text{Bob}) > dist(\text{Ada}, \text{Cathy})$? What if Jaccard similarity (Chapter 2) is used? What can you learn from this example?

11.3 Show that $I \times J$ is a bicluster with coherent values if and only if, for any $i_1, i_2 \in I$ and $j_1, j_2 \in J$, $e_{i_1 j_1} - e_{i_2 j_1} = e_{i_1 j_2} - e_{i_2 j_2}$.

11.4 Compare the MaPle algorithm (Section 11.2.3) with the frequent closed itemset mining algorithm, CLOSET (Pei, Han, and Mao [PHM00]). What are the major similarities and differences?

11.5 SimRank is a similarity measure for clustering graph and network data.

(a) Prove $\lim_{i \to \infty} s_i(u, v) = s(u, v)$ for SimRank computation.

(b) Show $s(u, v) = p(u, v)$ for SimRank.

11.6 In a large sparse graph where on average each node has a low degree, is the similarity matrix using SimRank still sparse? If so, in what sense? If not, why? Deliberate on your answer.

11.7 Compare the SCAN algorithm (Section 11.3.3) with DBSCAN (Section 10.4.1). What are their similarities and differences?

11.8 Consider partitioning clustering and the following constraint on clusters: The number of objects in each cluster must be between $\frac{n}{k}(1-\delta)$ and $\frac{n}{k}(1+\delta)$, where n is the total number of objects in the data set, k is the number of clusters desired, and δ in $[0, 1)$ is a parameter. Can you extend the k-means method to handle this constraint? Discuss situations where the constraint is hard and soft.

11.7 Bibliographic Notes

Höppner Klawonn, Kruse, and Runkler [HKKR99] provide a thorough discussion of fuzzy clustering. The fuzzy c-means algorithm (on which Example 11.7 is based) was proposed by Bezdek [Bez81]. Fraley and Raftery [FR02] give a comprehensive overview of model-based cluster analysis and probabilistic models. McLachlan and Basford [MB88] present a systematic introduction to mixture models and applications in cluster analysis.

Dempster, Laird, and Rubin [DLR77] are recognized as the first to introduce the EM algorithm and give it its name. However, the idea of the EM algorithm had been "proposed many times in special circumstances" before, as admitted in Dempster, Laird, and Rubin [DLR77]. Wu [Wu83] gives the correct analysis of the EM algorithm.

Mixture models and EM algorithms are used extensively in many data mining applications. Introductions to model-based clustering, mixture models, and EM algorithms can be found in recent textbooks on machine learning and statistical learning—for example, Bishop [Bis06], Marsland [Mar09], and Alpaydin [Alp11].

The increase of dimensionality has severe effects on distance functions, as indicated by Beyer et al. [BGRS99]. It also has had a dramatic impact on various techniques for classification, clustering, and semisupervised learning (Radovanović, Nanopoulos, and Ivanović [RNI09]).

Kriegel, Kröger, and Zimek [KKZ09] present a comprehensive survey on methods for clustering high-dimensional data. The CLIQUE algorithm was developed by Agrawal, Gehrke, Gunopulos, and Raghavan [AGGR98]. The PROCLUS algorithm was proposed by Aggawal, Procopiuc, Wolf, et al. [APW$^+$99].

The technique of biclustering was initially proposed by Hartigan [Har72]. The term *biclustering* was coined by Mirkin [Mir98]. Cheng and Church [CC00] introduced biclustering into gene expression data analysis. There are many studies on biclustering models and methods. The notion of δ-pCluster was introduced by Wang, Wang, Yang, and Yu [WWYY02]. For informative surveys, see Madeira and Oliveira [MO04] and Tanay, Sharan, and Shamir [TSS04]. In this chapter, we introduced the δ-cluster algorithm by Cheng and Church [CC00] and MaPle by Pei, Zhang, Cho, et al. [PZC$^+$03] as examples of optimization-based methods and enumeration methods for biclustering, respectively.

Donath and Hoffman [DH73] and Fiedler [Fie73] pioneered spectral clustering. In this chapter, we use an algorithm proposed by Ng, Jordan, and Weiss [NJW01] as an example. For a thorough tutorial on spectral clustering, see Luxburg [Lux07].

Clustering graph and network data is an important and fast-growing topic. Schaeffer [Sch07] provides a survey. The SimRank measure of similarity was developed by Jeh and Widom [JW02a]. Xu et al. [XYFS07] proposed the SCAN algorithm. Arora, Rao, and Vazirani [ARV09] discuss the sparsest cuts and approximation algorithms.

Clustering with constraints has been extensively studied. Davidson, Wagstaff, and Basu [DWB06] proposed the measures of informativeness and coherence. The COP-k-means algorithm is given by Wagstaff et al. [WCRS01]. The CVQE algorithm was proposed by Davidson and Ravi [DR05]. Tung, Han, Lakshmanan, and Ng [THLN01] presented a framework for constraint-based clustering based on user-specified constraints. An efficient method for constraint-based spatial clustering in the existence of physical obstacle constraints was proposed by Tung, Hou, and Han [THH01].

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12 Outlier Detection

Imagine that you are a transaction auditor in a credit card company. To protect your customers from credit card fraud, you pay special attention to card usages that are rather different from typical cases. For example, if a purchase amount is much bigger than usual for a card owner, and if the purchase occurs far from the owner's resident city, then the purchase is suspicious. You want to detect such transactions as soon as they occur and contact the card owner for verification. This is common practice in many credit card companies. *What data mining techniques can help detect suspicious transactions?*

Most credit card transactions are normal. However, if a credit card is stolen, its transaction pattern usually changes dramatically—the locations of purchases and the items purchased are often very different from those of the authentic card owner and other customers. An essential idea behind credit card fraud detection is to identify those transactions that are very different from the norm.

Outlier detection (also known as *anomaly detection*) is the process of finding data objects with behaviors that are very different from expectation. Such objects are called **outliers** or **anomalies**. Outlier detection is important in many applications in addition to fraud detection such as medical care, public safety and security, industry damage detection, image processing, sensor/video network surveillance, and intrusion detection.

Outlier detection and clustering analysis are two highly related tasks. Clustering finds the majority patterns in a data set and organizes the data accordingly, whereas outlier detection tries to capture those exceptional cases that deviate substantially from the majority patterns. Outlier detection and clustering analysis serve different purposes.

In this chapter, we study outlier detection techniques. Section 12.1 defines the different types of outliers. Section 12.2 presents an overview of outlier detection methods. In the rest of the chapter, you will learn about outlier detection methods in detail. These approaches, organized here by category, are statistical (Section 12.3), proximity-based (Section 12.4), clustering-based (Section 12.5), and classification-based (Section 12.6). In addition, you will learn about mining contextual and collective outliers (Section 12.7) and outlier detection in high-dimensional data (Section 12.8).

12.1 Outliers and Outlier Analysis

Let us first define what outliers are, categorize the different types of outliers, and then discuss the challenges in outlier detection at a general level.

12.1.1 What Are Outliers?

Assume that a given statistical process is used to generate a set of data objects. An **outlier** is a data object that deviates significantly from the rest of the objects, as if it were generated by a different mechanism. For ease of presentation within this chapter, we may refer to data objects that are not outliers as "normal" or expected data. Similarly, we may refer to outliers as "abnormal" data.

Example 12.1 **Outliers.** In Figure 12.1, most objects follow a roughly Gaussian distribution. However, the objects in region *R* are significantly different. It is unlikely that they follow the same distribution as the other objects in the data set. Thus, the objects in *R* are outliers in the data set. ■

Outliers are different from noisy data. As mentioned in Chapter 3, noise is a random error or variance in a measured variable. In general, noise is not interesting in data analysis, including outlier detection. For example, in credit card fraud detection, a customer's purchase behavior can be modeled as a random variable. A customer may generate some "noise transactions" that may seem like "random errors" or "variance," such as by buying a bigger lunch one day, or having one more cup of coffee than usual. Such transactions should not be treated as outliers; otherwise, the credit card company would incur heavy costs from verifying that many transactions. The company may also lose customers by bothering them with multiple false alarms. As in many other data analysis and data mining tasks, noise should be removed before outlier detection.

Outliers are interesting because they are suspected of not being generated by the same mechanisms as the rest of the data. Therefore, in outlier detection, it is important to

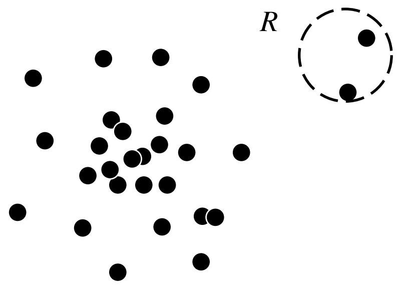


Figure 12.1 The objects in region *R* are outliers.

justify *why* the outliers detected are generated by some other mechanisms. This is often achieved by making various assumptions on the rest of the data and showing that the outliers detected violate those assumptions significantly.

Outlier detection is also related to *novelty detection* in evolving data sets. For example, by monitoring a social media web site where new content is incoming, novelty detection may identify new topics and trends in a timely manner. Novel topics may initially appear as outliers. To this extent, outlier detection and novelty detection share some similarity in modeling and detection methods. However, a critical difference between the two is that in novelty detection, once new topics are confirmed, they are usually incorporated into the model of normal behavior so that follow-up instances are not treated as outliers anymore.

12.1.2 Types of Outliers

In general, outliers can be classified into three categories, namely global outliers, contextual (or conditional) outliers, and collective outliers. Let's examine each of these categories.

Global Outliers

In a given data set, a data object is a **global outlier** if it deviates significantly from the rest of the data set. Global outliers are sometimes called *point anomalies*, and are the simplest type of outliers. Most outlier detection methods are aimed at finding global outliers.

Example 12.2 **Global outliers.** Consider the points in Figure 12.1 again. The points in region R significantly deviate from the rest of the data set, and hence are examples of global outliers. ■

To detect global outliers, a critical issue is to find an appropriate measurement of deviation with respect to the application in question. Various measurements are proposed, and, based on these, outlier detection methods are partitioned into different categories. We will come to this issue in detail later.

Global outlier detection is important in many applications. Consider intrusion detection in computer networks, for example. If the communication behavior of a computer is very different from the normal patterns (e.g., a large number of packages is broadcast in a short time), this behavior may be considered as a global outlier and the corresponding computer is a suspected victim of hacking. As another example, in trading transaction auditing systems, transactions that do not follow the regulations are considered as global outliers and should be held for further examination.

Contextual Outliers

"The temperature today is 28° *C. Is it exceptional (i.e., an outlier)?"* It depends, for example, on the time and location! If it is in winter in Toronto, yes, it is an outlier. If it is a summer day in Toronto, then it is normal. Unlike global outlier detection, in this case,

whether or not today's temperature value is an outlier depends on the context—the date, the location, and possibly some other factors.

In a given data set, a data object is a **contextual outlier** if it deviates significantly with respect to a specific context of the object. Contextual outliers are also known as *conditional outliers* because they are conditional on the selected context. Therefore, in contextual outlier detection, the context has to be specified as part of the problem definition. Generally, in contextual outlier detection, the attributes of the data objects in question are divided into two groups:

- **Contextual attributes**: The contextual attributes of a data object define the object's context. In the temperature example, the contextual attributes may be date and location.
- **Behavioral attributes**: These define the object's characteristics, and are used to evaluate whether the object is an outlier in the context to which it belongs. In the temperature example, the behavioral attributes may be the temperature, humidity, and pressure.

Unlike global outlier detection, in contextual outlier detection, whether a data object is an outlier depends on not only the behavioral attributes but also the contextual attributes. A configuration of behavioral attribute values may be considered an outlier in one context (e.g., 28°C is an outlier for a Toronto winter), but not an outlier in another context (e.g., 28°C is not an outlier for a Toronto summer).

Contextual outliers are a generalization of local outliers, a notion introduced in density-based outlier analysis approaches. An object in a data set is a **local outlier** if its density significantly deviates from the local area in which it occurs. We will discuss local outlier analysis in greater detail in Section 12.4.3.

Global outlier detection can be regarded as a special case of contextual outlier detection where the set of contextual attributes is empty. In other words, global outlier detection uses the whole data set as the context. Contextual outlier analysis provides flexibility to users in that one can examine outliers in different contexts, which can be highly desirable in many applications.

Example 12.3 **Contextual outliers.** In credit card fraud detection, in addition to global outliers, an analyst may consider outliers in different contexts. Consider customers who use more than 90% of their credit limit. If one such customer is viewed as belonging to a group of customers with low credit limits, then such behavior may not be considered an outlier. However, similar behavior of customers from a high-income group may be considered outliers if their balance often exceeds their credit limit. Such outliers may lead to business opportunities—raising credit limits for such customers can bring in new revenue. ■

The quality of contextual outlier detection in an application depends on the meaningfulness of the contextual attributes, in addition to the measurement of the deviation of an object to the majority in the space of behavioral attributes. More often than not, the contextual attributes should be determined by domain experts, which can be regarded as part of the input background knowledge. In many applications, neither obtaining sufficient information to determine contextual attributes nor collecting high-quality contextual attribute data is easy.

"How can we formulate meaningful contexts in contextual outlier detection?" A straightforward method simply uses group-bys of the contextual attributes as contexts. This may not be effective, however, because many group-bys may have insufficient data and/or noise. A more general method uses the proximity of data objects in the space of contextual attributes. We discuss this approach in detail in Section 12.4.

Collective Outliers

Suppose you are a supply-chain manager of *AllElectronics*. You handle thousands of orders and shipments every day. If the shipment of an order is delayed, it may not be considered an outlier because, statistically, delays occur from time to time. However, you have to pay attention if 100 orders are delayed on a single day. Those 100 orders as a whole form an outlier, although each of them may not be regarded as an outlier if considered individually. You may have to take a close look at those orders collectively to understand the shipment problem.

Given a data set, a subset of data objects forms a **collective outlier** if the objects as a whole deviate significantly from the entire data set. Importantly, the individual data objects may not be outliers.

Example 12.4 **Collective outliers.** In Figure 12.2, the black objects as a whole form a collective outlier because the density of those objects is much higher than the rest in the data set. However, every black object individually is not an outlier with respect to the whole data set.

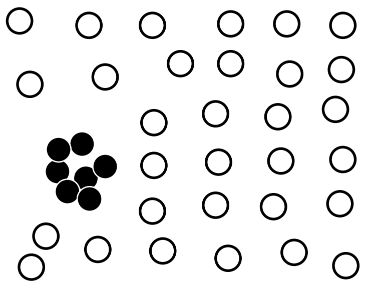


Figure 12.2 The black objects form a collective outlier. ■

Collective outlier detection has many important applications. For example, in intrusion detection, a denial-of-service package from one computer to another is considered normal, and not an outlier at all. However, if several computers keep sending denial-of-service packages to each other, they as a whole should be considered as a collective outlier. The computers involved may be suspected of being compromised by an attack. As another example, a stock transaction between two parties is considered normal. However, a large set of transactions of the same stock among a small party in a short period are collective outliers because they may be evidence of some people manipulating the market.

Unlike global or contextual outlier detection, in collective outlier detection we have to consider not only the behavior of individual objects, but also that of groups of objects. Therefore, to detect collective outliers, we need background knowledge of the relationship among data objects such as distance or similarity measurements between objects.

In summary, a data set can have multiple types of outliers. Moreover, an object may belong to more than one type of outlier. In business, different outliers may be used in various applications or for different purposes. Global outlier detection is the simplest. Context outlier detection requires background information to determine contextual attributes and contexts. Collective outlier detection requires background information to model the relationship among objects to find groups of outliers.

12.1.3 Challenges of Outlier Detection

Outlier detection is useful in many applications yet faces many challenges such as the following:

- **Modeling normal objects and outliers effectively.** Outlier detection quality highly depends on the modeling of normal (nonoutlier) objects and outliers. Often, building a comprehensive model for data normality is very challenging, if not impossible. This is partly because it is hard to enumerate all possible normal behaviors in an application.

  The border between data normality and abnormality (outliers) is often not clear cut. Instead, there can be a wide range of gray area. Consequently, while some outlier detection methods assign to each object in the input data set a label of either "normal" or "outlier," other methods assign to each object a score measuring the "outlier-ness" of the object.

- **Application-specific outlier detection.** Technically, choosing the similarity/distance measure and the relationship model to describe data objects is critical in outlier detection. Unfortunately, such choices are often application-dependent. Different applications may have very different requirements. For example, in clinic data analysis, a small deviation may be important enough to justify an outlier. In contrast, in marketing analysis, objects are often subject to larger fluctuations, and consequently a substantially larger deviation is needed to justify an outlier. Outlier detection's high dependency on the application type makes it impossible to develop a universally applicable outlier detection method. Instead, individual outlier detection methods that are dedicated to specific applications must be developed.

- **Handling noise in outlier detection.** As mentioned earlier, outliers are different from noise. It is also well known that the quality of real data sets tends to be poor. Noise often unavoidably exists in data collected in many applications. Noise may be present as deviations in attribute values or even as missing values. Low data quality and the presence of noise bring a huge challenge to outlier detection. They can distort the data, blurring the distinction between normal objects and outliers. Moreover, noise and missing data may "hide" outliers and reduce the effectiveness of outlier detection—an outlier may appear "disguised" as a noise point, and an outlier detection method may mistakenly identify a noise point as an outlier.
- **Understandability.** In some application scenarios, a user may want to not only detect outliers, but also understand why the detected objects are outliers. To meet the understandability requirement, an outlier detection method has to provide some justification of the detection. For example, a statistical method can be used to justify the degree to which an object may be an outlier based on the likelihood that the object was generated by the same mechanism that generated the majority of the data. The smaller the likelihood, the more unlikely the object was generated by the same mechanism, and the more likely the object is an outlier.

The rest of this chapter discusses approaches to outlier detection.

12.2 Outlier Detection Methods

There are many outlier detection methods in the literature and in practice. Here, we present two orthogonal ways to categorize outlier detection methods. First, we categorize outlier detection methods according to whether the sample of data for analysis is given with domain expert–provided labels that can be used to build an outlier detection model. Second, we divide methods into groups according to their assumptions regarding normal objects versus outliers.

12.2.1 Supervised, Semi-Supervised, and Unsupervised Methods

If expert-labeled examples of normal and/or outlier objects can be obtained, they can be used to build outlier detection models. The methods used can be divided into supervised methods, semi-supervised methods, and unsupervised methods.

Supervised Methods

Supervised methods model data normality and abnormality. Domain experts examine and label a sample of the underlying data. Outlier detection can then be modeled as a classification problem (Chapters 8 and 9). The task is to learn a classifier that can recognize outliers. The sample is used for training and testing. In some applications, the experts may label just the normal objects, and any other objects not matching the model of normal objects are reported as outliers. Other methods model the outliers and treat objects not matching the model of outliers as normal.

Although many classification methods can be applied, challenges to supervised outlier detection include the following:

- The two classes (i.e., normal objects versus outliers) are imbalanced. That is, the population of outliers is typically much smaller than that of normal objects. Therefore, methods for handling imbalanced classes (Section 8.6.5) may be used, such as oversampling (i.e., replicating) outliers to increase their distribution in the training set used to construct the classifier. Due to the small population of outliers in data, the sample data examined by domain experts and used in training may not even sufficiently represent the outlier distribution. The lack of outlier samples can limit the capability of classifiers built as such. To tackle these problems, some methods "make up" artificial outliers.
- In many outlier detection applications, catching as many outliers as possible (i.e., the sensitivity or recall of outlier detection) is far more important than not mislabeling normal objects as outliers. Consequently, when a classification method is used for supervised outlier detection, it has to be interpreted appropriately so as to consider the application interest on recall.

In summary, supervised methods of outlier detection must be careful in how they train and how they interpret classification rates due to the fact that outliers are rare in comparison to the other data samples.

Unsupervised Methods

In some application scenarios, objects labeled as "normal" or "outlier" are not available. Thus, an unsupervised learning method has to be used.

Unsupervised outlier detection methods make an implicit assumption: The normal objects are somewhat "clustered." In other words, an unsupervised outlier detection method expects that normal objects follow a pattern far more frequently than outliers. Normal objects do not have to fall into one group sharing high similarity. Instead, they can form multiple groups, where each group has distinct features. However, an outlier is expected to occur far away in feature space from any of those groups of normal objects.

This assumption may not be true all the time. For example, in Figure 12.2, the normal objects do not share any strong patterns. Instead, they are uniformly distributed. The collective outliers, however, share high similarity in a small area. Unsupervised methods cannot detect such outliers effectively. In some applications, normal objects are diversely distributed, and many such objects do not follow strong patterns. For instance, in some intrusion detection and computer virus detection problems, normal activities are very diverse and many do not fall into high-quality clusters. In such scenarios, unsupervised methods may have a high false positive rate—they may mislabel many normal objects as outliers (intrusions or viruses in these applications), and let many actual outliers go undetected. Due to the high similarity between intrusions and viruses (i.e., they have to attack key resources in the target systems), modeling outliers using supervised methods may be far more effective.

Many clustering methods can be adapted to act as unsupervised outlier detection methods. The central idea is to find clusters first, and then the data objects not belonging to any cluster are detected as outliers. However, such methods suffer from two issues. First, a data object not belonging to any cluster may be noise instead of an outlier. Second, it is often costly to find clusters first and then find outliers. It is usually assumed that there are far fewer outliers than normal objects. Having to process a large population of nontarget data entries (i.e., the normal objects) before one can touch the real meat (i.e., the outliers) can be unappealing. The latest unsupervised outlier detection methods develop various smart ideas to tackle outliers directly without explicitly and completely finding clusters. You will learn more about these techniques in Sections 12.4 and 12.5 on proximity-based and clustering-based methods, respectively.

Semi-Supervised Methods

In many applications, although obtaining some labeled examples is feasible, the number of such labeled examples is often small. We may encounter cases where only a small set of the normal and/or outlier objects are labeled, but most of the data are unlabeled. Semi-supervised outlier detection methods were developed to tackle such scenarios.

Semi-supervised outlier detection methods can be regarded as applications of semi-supervised learning methods (Section 9.7.2). For example, when some labeled normal objects are available, we can use them, together with unlabeled objects that are close by, to train a model for normal objects. The model of normal objects then can be used to detect outliers—those objects not fitting the model of normal objects are classified as outliers.

If only some labeled outliers are available, semi-supervised outlier detection is trickier. A small number of labeled outliers are unlikely to represent all the possible outliers. Therefore, building a model for outliers based on only a few labeled outliers is unlikely to be effective. To improve the quality of outlier detection, we can get help from models for normal objects learned from unsupervised methods.

For additional information on semi-supervised methods, interested readers are referred to the bibliographic notes at the end of this chapter (Section 12.11).

12.2.2 Statistical Methods, Proximity-Based Methods, and Clustering-Based Methods

As discussed in Section 12.1, outlier detection methods make assumptions about outliers versus the rest of the data. According to the assumptions made, we can categorize outlier detection methods into three types: statistical methods, proximity-based methods, and clustering-based methods.

Statistical Methods

Statistical methods (also known as **model-based methods**) make assumptions of data normality. They assume that normal data objects are generated by a statistical (stochastic) model, and that data not following the model are outliers.

Example 12.5 **Detecting outliers using a statistical (Gaussian) model.** In Figure 12.1, the data points except for those in region R fit a Gaussian distribution g_D, where for a location $\boldsymbol{x}$ in the data space, $g_D(\boldsymbol{x})$ gives the probability density at $\boldsymbol{x}$. Thus, the Gaussian distribution g_D can be used to model the normal data, that is, most of the data points in the data set. For each object $\boldsymbol{y}$ in region, R, we can estimate $g_D(\boldsymbol{y})$, the probability that this point fits the Gaussian distribution. Because $g_D(\boldsymbol{y})$ is very low, $\boldsymbol{y}$ is unlikely generated by the Gaussian model, and thus is an outlier. ■

The effectiveness of statistical methods highly depends on whether the assumptions made for the statistical model hold true for the given data. There are many kinds of statistical models. For example, the statistic models used in the methods may be parametric or nonparametric. Statistical methods for outlier detection are discussed in detail in Section 12.3.

Proximity-Based Methods

Proximity-based methods assume that an object is an outlier if the nearest neighbors of the object are far away in feature space, that is, the proximity of the object to its neighbors significantly deviates from the proximity of most of the other objects to their neighbors in the same data set.

Example 12.6 **Detecting outliers using proximity.** Consider the objects in Figure 12.1 again. If we model the proximity of an object using its three nearest neighbors, then the objects in region R are substantially different from other objects in the data set. For the two objects in R, their second and third nearest neighbors are dramatically more remote than those of any other objects. Therefore, we can label the objects in R as outliers based on proximity. ■

The effectiveness of proximity-based methods relies heavily on the proximity (or distance) measure used. In some applications, such measures cannot be easily obtained. Moreover, proximity-based methods often have difficulty in detecting a group of outliers if the outliers are close to one another.

There are two major types of proximity-based outlier detection, namely *distance-based* and *density-based* outlier detection. Proximity-based outlier detection is discussed in Section 12.4.

Clustering-Based Methods

Clustering-based methods assume that the normal data objects belong to large and dense clusters, whereas outliers belong to small or sparse clusters, or do not belong to any clusters.

Example 12.7 **Detecting outliers using clustering.** In Figure 12.1, there are two clusters. Cluster C_1 contains all the points in the data set except for those in region R. Cluster C_2 is tiny, containing just two points in R. Cluster C_1 is large in comparison to C_2. Therefore, a clustering-based method asserts that the two objects in R are outliers. ■

There are many clustering methods, as discussed in Chapters 10 and 11. Therefore, there are many clustering-based outlier detection methods as well. Clustering is an expensive data mining operation. A straightforward adaptation of a clustering method for outlier detection can be very costly, and thus does not scale up well for large data sets. Clustering-based outlier detection methods are discussed in detail in Section 12.5.

12.3 Statistical Approaches

As with statistical methods for clustering, statistical methods for outlier detection make assumptions about data normality. They assume that the normal objects in a data set are generated by a stochastic process (a generative model). Consequently, normal objects occur in regions of high probability for the stochastic model, and objects in the regions of low probability are outliers.

The general idea behind statistical methods for outlier detection is to learn a generative model fitting the given data set, and then identify those objects in low-probability regions of the model as outliers. However, there are many different ways to learn generative models. In general, statistical methods for outlier detection can be divided into two major categories: *parametric methods* and *nonparametric methods*, according to how the models are specified and learned.

A **parametric method** assumes that the normal data objects are generated by a parametric distribution with parameter Θ. The *probability density function* of the parametric distribution $f(\boldsymbol{x}, \Theta)$ gives the probability that object $\boldsymbol{x}$ is generated by the distribution. The smaller this value, the more likely $\boldsymbol{x}$ is an outlier.

A **nonparametric method** does not assume an a priori statistical model. Instead, a nonparametric method tries to determine the model from the input data. Note that most nonparametric methods do not assume that the model is completely parameter-free. (Such an assumption would make learning the model from data almost mission impossible.) Instead, nonparametric methods often take the position that the number and nature of the parameters are flexible and not fixed in advance. Examples of nonparametric methods include histogram and kernel density estimation.

12.3.1 Parametric Methods

In this subsection, we introduce several simple yet practical parametric methods for outlier detection. We first discuss methods for univariate data based on normal distribution. We then discuss how to handle multivariate data using multiple parametric distributions.

Detection of Univariate Outliers Based on Normal Distribution

Data involving only one attribute or variable are called *univariate data.* For simplicity, we often choose to assume that data are generated from a normal distribution. We can then learn the parameters of the normal distribution from the input data, and identify the points with low probability as outliers.

Let's start with univariate data. We will try to detect outliers by assuming the data follow a normal distribution.

Example 12.8 **Univariate outlier detection using maximum likelihood.** Suppose a city's average temperature values in July in the last 10 years are, in value-ascending order, 24.0°C, 28.9°C, 28.9°C, 29.0°C, 29.1°C, 29.1°C, 29.2°C, 29.2°C, 29.3°C, and 29.4°C. Let's assume that the average temperature follows a normal distribution, which is determined by two parameters: the mean, μ, and the standard deviation, σ.

We can use the *maximum likelihood method* to estimate the parameters μ and σ. That is, we maximize the *log-likelihood function*

$$\ln \mathcal{L}(\mu,\sigma^2) = \sum_{i=1}^{n} \ln f(x_i|(\mu,\sigma^2)) = -\frac{n}{2}\ln(2\pi) - \frac{n}{2}\ln\sigma^2 - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2, \quad (12.1)$$

where n is the total number of samples, which is 10 in this example.

Taking derivatives with respect to μ and σ^2 and solving the resulting system of first-order conditions leads to the following *maximum likelihood estimates*:

$$\hat{\mu} = \overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \quad (12.2)$$

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \overline{x})^2. \quad (12.3)$$

In this example, we have

$$\hat{\mu} = \frac{24.0+28.9+28.9+29.0+29.1+29.1+29.2+29.2+29.3+29.4}{10} = 28.61$$

$$\begin{aligned}\hat{\sigma}^2 = &((24.1-28.61)^2+(28.9-28.61)^2+(28.9-28.61)^2+(29.0-28.61)^2\\ &+(29.1-28.61)^2+(29.1-28.61)^2+(29.2-28.61)^2+(29.2-28.61)^2\\ &+(29.3-28.61)^2+(29.4-28.61)^2)/10 \backsimeq 2.29.\end{aligned}$$

Accordingly, we have $\hat{\sigma} = \sqrt{2.29} = 1.51$.

The most deviating value, 24.0°C, is 4.61°C away from the estimated mean. We know that the $\mu \pm 3\sigma$ region contains 99.7% data under the assumption of normal

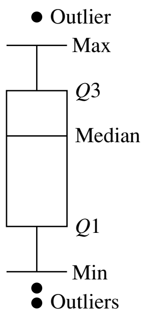


Figure 12.3 Using a boxplot to visualize outliers.

distribution. Because $\frac{4.61}{1.51} = 3.04 > 3$, the probability that the value 24.0°C is generated by the normal distribution is less than 0.15%, and thus can be identified as an outlier. ■

Example 12.8 elaborates a simple yet practical outlier detection method. It simply labels any object as an outlier if it is more than 3σ away from the mean of the estimated distribution, where σ is the standard deviation.

Such straightforward methods for statistical outlier detection can also be used in visualization. For example, the *boxplot method* (described in Chapter 2) plots the univariate input data using a five-number summary (Figure 12.3): the smallest nonoutlier value (Min), the lower quartile ($Q1$), the median ($Q2$), the upper quartile ($Q3$), and the largest nonoutlier value (Max). The *interquantile range* (*IQR*) is defined as $Q3 - Q1$. Any object that is more than $1.5 \times IQR$ smaller than $Q1$ or $1.5 \times IQR$ larger than $Q3$ is treated as an outlier because the region between $Q1 - 1.5 \times IQR$ and $Q3 + 1.5 \times IQR$ contains 99.3% of the objects. The rationale is similar to using 3σ as the threshold for normal distribution.

Another simple statistical method for univariate outlier detection using normal distribution is the *Grubb's test* (also known as the *maximum normed residual test*). For each object x in a data set, we define a z-score as

$$z = \frac{|x - \bar{x}|}{s}, \tag{12.4}$$

where $\bar{x}$ is the mean, and s is the standard deviation of the input data. An object x is an outlier if

$$z \geq \frac{N-1}{\sqrt{N}} \sqrt{\frac{t^2_{\alpha/(2N),N-2}}{N-2+t^2_{\alpha/(2N),N-2}}}, \tag{12.5}$$

where $t^2_{\alpha/(2N),N-2}$ is the value taken by a t-distribution at a significance level of $\alpha/(2N)$, and N is the number of objects in the data set.

Detection of Multivariate Outliers

Data involving two or more attributes or variables are *multivariate data.* Many univariate outlier detection methods can be extended to handle multivariate data. The central idea is to transform the multivariate outlier detection task into a univariate outlier detection problem. Here, we use two examples to illustrate this idea.

Example 12.9 Multivariate outlier detection using the Mahalanobis distance. For a multivariate data set, let $\bar{\boldsymbol{o}}$ be the mean vector. For an object, $\boldsymbol{o}$, in the data set, the Mahalanobis distance from $\boldsymbol{o}$ to $\bar{\boldsymbol{o}}$ is

$$MDist(\boldsymbol{o},\bar{\boldsymbol{o}}) = (\boldsymbol{o}-\bar{\boldsymbol{o}})^T S^{-1}(\boldsymbol{o}-\bar{\boldsymbol{o}}), \tag{12.6}$$

where S is the covariance matrix.

$MDist(\boldsymbol{o},\bar{\boldsymbol{o}})$ is a univariate variable, and thus Grubb's test can be applied to this measure. Therefore, we can transform the multivariate outlier detection tasks as follows:

1. Calculate the mean vector from the multivariate data set.
2. For each object $\boldsymbol{o}$, calculate $MDist(\boldsymbol{o},\bar{\boldsymbol{o}})$, the Mahalanobis distance from $\boldsymbol{o}$ to $\bar{\boldsymbol{o}}$.
3. Detect outliers in the transformed univariate data set, $\{MDist(\boldsymbol{o},\bar{\boldsymbol{o}}) | \boldsymbol{o} \in D\}$.
4. If $MDist(\boldsymbol{o},\bar{\boldsymbol{o}})$ is determined to be an outlier, then $\boldsymbol{o}$ is regarded as an outlier as well.

■

Our second example uses the χ^2-statistic to measure the distance between an object to the mean of the input data set.

Example 12.10 Multivariate outlier detection using the χ^2-statistic. The χ^2-statistic can also be used to capture multivariate outliers under the assumption of normal distribution. For an object, $\boldsymbol{o}$, the χ^2-statistic is

$$\chi^2 = \sum_{i=1}^{n} \frac{(o_i - E_i)^2}{E_i}, \tag{12.7}$$

where $\boldsymbol{o}_i$ is the value of $\boldsymbol{o}$ on the ith dimension, E_i is the mean of the i-dimension among all objects, and n is the dimensionality. If the χ^2-statistic is large, the object is an outlier. ■

Using a Mixture of Parametric Distributions

If we assume that the data were generated by a normal distribution, this works well in many situations. However, this assumption may be overly simplified when the actual data distribution is complex. In such cases, we instead assume that the data were generated by a mixture of parametric distributions.

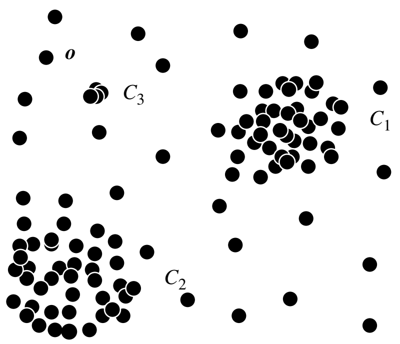


Figure 12.4 A complex data set.

Example 12.11 **Multivariate outlier detection using multiple parametric distributions.** Consider the data set in Figure 12.4. There are two big clusters, C_1 and C_2. To assume that the data are generated by a normal distribution would not work well here. The estimated mean is located between the two clusters and not inside any cluster. The objects between the two clusters cannot be detected as outliers since they are close to the mean. ■

To overcome this problem, we can instead assume that the normal data objects are generated by multiple normal distributions, two in this case. That is, we assume two normal distributions, $\Theta_1(\mu_1,\sigma_1)$ and $\Theta_2(\mu_2,\sigma_2)$. For any object, $\boldsymbol{o}$, in the data set, the probability that $\boldsymbol{o}$ is generated by the mixture of the two distributions is given by

$$Pr(\boldsymbol{o}|\Theta_1,\Theta_2) = f_{\Theta_1}(\boldsymbol{o}) + f_{\Theta_2}(\boldsymbol{o}),$$

where f_{Θ_1} and f_{Θ_2} are the probability density functions of Θ_1 and Θ_2, respectively. We can use the *expectation-maximization* (EM) algorithm (Chapter 11) to learn the parameters $\mu_1,\sigma_1,\mu_2,\sigma_2$ from the data, as we do in mixture models for clustering. Each cluster is represented by a learned normal distribution. An object, $\boldsymbol{o}$, is detected as an outlier if it does not belong to any cluster, that is, the probability is very low that it was generated by the combination of the two distributions.

Example 12.12 **Multivariate outlier detection using multiple clusters.** Most of the data objects shown in Figure 12.4 are in either C_1 or C_2. Other objects, representing noise, are uniformly distributed in the data space. A small cluster, C_3, is highly suspicious because it is not close to either of the two major clusters, C_1 and C_2. The objects in C_3 should therefore be detected as outliers.

Note that identifying the objects in C_3 as outliers is difficult, whether or not we assume that the given data follow a normal distribution or a mixture of multiple distributions. This is because the probability of the objects in C_3 will be higher than some of the noise objects, like $\boldsymbol{o}$ in Figure 12.4, due to a higher local density in C_3. ■

To tackle the problem demonstrated in Example 12.12, we can assume that the normal data objects are generated by a normal distribution, or a mixture of normal distributions, whereas the outliers are generated by another distribution. Heuristically, we can add constraints on the distribution that is generating outliers. For example, it is reasonable to assume that this distribution has a larger variance if the outliers are distributed in a larger area. Technically, we can assign $\sigma_{outlier} = k\sigma$, where k is a user-specified parameter and σ is the standard deviation of the normal distribution generating the normal data. Again, the EM algorithm can be used to learn the parameters.

12.3.2 Nonparametric Methods

In nonparametric methods for outlier detection, the model of "normal data" is learned from the input data, rather than assuming one a priori. Nonparametric methods often make fewer assumptions about the data, and thus can be applicable in more scenarios.

Example 12.13 **Outlier detection using a histogram.** *AllElectronics* records the purchase amount for every customer transaction. Figure 12.5 uses a histogram (refer to Chapters 2 and 3) to graph these amounts as percentages, given all transactions. For example, 60% of the transaction amounts are between \$0.00 and \$1000.

We can use the histogram as a nonparametric statistical model to capture outliers. For example, a transaction in the amount of \$7500 can be regarded as an outlier because only $1 - (60\% + 20\% + 10\% + 6.7\% + 3.1\%) = 0.2\%$ of transactions have an amount higher than \$5000. On the other hand, a transaction amount of \$385 can be treated as normal because it falls into the bin (or bucket) holding 60% of the transactions.

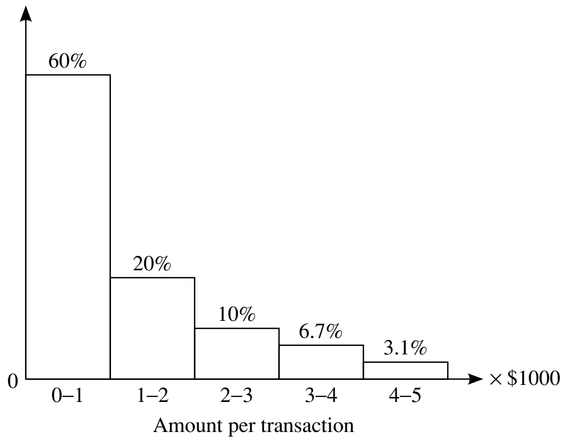


Figure 12.5 Histogram of purchase amounts in transactions.

■

As illustrated in the previous example, the histogram is a frequently used nonparametric statistical model that can be used to detect outliers. The procedure involves the following two steps.

Step 1: Histogram construction. In this step, we construct a histogram using the input data (training data). The histogram may be univariate as in Example 12.13, or multivariate if the input data are multidimensional.

Note that although nonparametric methods do not assume any a priori statistical model, they often do require user-specified parameters to learn models from data. For example, to construct a good histogram, a user has to specify the type of histogram (e.g., equal width or equal depth) and other parameters (e.g., the number of bins in the histogram or the size of each bin). Unlike parametric methods, these parameters do not specify types of data distribution (e.g., Gaussian).

Step 2: Outlier detection. To determine whether an object, $\boldsymbol{o}$, is an outlier, we can check it against the histogram. In the simplest approach, if the object falls in one of the histogram's bins, the object is regarded as normal. Otherwise, it is considered an outlier.

For a more sophisticated approach, we can use the histogram to assign an outlier score to the object. In Example 12.13, we can let an object's outlier score be the inverse of the volume of the bin in which the object falls. For example, the outlier score for a transaction amount of \$7500 is $\frac{1}{0.2\%} = 500$, and that for a transaction amount of \$385 is $\frac{1}{60\%} = 1.67$. The scores indicate that the transaction amount of \$7500 is much more likely to be an outlier than that of \$385.

A drawback to using histograms as a nonparametric model for outlier detection is that it is hard to choose an appropriate bin size. On the one hand, if the bin size is set too small, many normal objects may end up in empty or rare bins, and thus be misidentified as outliers. This leads to a high false positive rate and low precision. On the other hand, if the bin size is set too high, outlier objects may infiltrate into some frequent bins and thus be "disguised" as normal. This leads to a high false negative rate and low recall.

To overcome this problem, we can adopt kernel density estimation to estimate the probability density distribution of the data. We treat an observed object as an indicator of high probability density in the surrounding region. The probability density at a point depends on the distances from this point to the observed objects. We use a *kernel function* to model the influence of a sample point within its neighborhood. A kernel $K()$ is a non-negative real-valued integrable function that satisfies the following two conditions:

- $\int_{-\infty}^{+\infty} K(u)du = 1$.
- $K(-u) = K(u)$ for all values of u.

A frequently used kernel is a standard Gaussian function with mean 0 and variance 1:

$$K\left(\frac{x - x_i}{h}\right) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_i)^2}{2h^2}}. \tag{12.8}$$

Let $x_1, \ldots, x_n$ be an independent and identically distributed sample of a random variable f. The kernel density approximation of the probability density function is

$$\hat{f}_h(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right), \tag{12.9}$$

where $K()$ is a kernel and h is the bandwidth serving as a smoothing parameter.

Once the probability density function of a data set is approximated through kernel density estimation, we can use the estimated density function $\hat{f}$ to detect outliers. For an object, o, $\hat{f}(o)$ gives the estimated probability that the object is generated by the stochastic process. If $\hat{f}(o)$ is high, then the object is likely normal. Otherwise, o is likely an outlier. This step is often similar to the corresponding step in parametric methods.

In summary, statistical methods for outlier detection learn models from data to distinguish normal data objects from outliers. An advantage of using statistical methods is that the outlier detection may be statistically justifiable. Of course, this is true only if the statistical assumption made about the underlying data meets the constraints in reality.

The data distribution of high-dimensional data is often complicated and hard to fully understand. Consequently, statistical methods for outlier detection on high-dimensional data remain a big challenge. Outlier detection for high-dimensional data is further addressed in Section 12.8.

The computational cost of statistical methods depends on the models. When simple parametric models are used (e.g., a Gaussian), fitting the parameters typically takes linear time. When more sophisticated models are used (e.g., mixture models, where the EM algorithm is used in learning), approximating the best parameter values often takes several iterations. Each iteration, however, is typically linear with respect to the data set's size. For kernel density estimation, the model learning cost can be up to quadratic. Once the model is learned, the outlier detection cost is often very small per object.

12.4 Proximity-Based Approaches

Given a set of objects in feature space, a distance measure can be used to quantify the similarity between objects. Intuitively, objects that are far from others can be regarded as outliers. Proximity-based approaches assume that the proximity of an outlier object to its nearest neighbors significantly deviates from the proximity of the object to most of the other objects in the data set.

There are two types of proximity-based outlier detection methods: distance-based and density-based methods. A *distance-based outlier detection method* consults the **neighborhood** of an object, which is defined by a given radius. An object is then considered an outlier if its neighborhood does not have enough other points. A *density-based outlier detection method* investigates the density of an object and that of its neighbors. Here, an object is identified as an outlier if its density is relatively much lower than that of its neighbors.

Let's start with distance-based outliers.

12.4.1 Distance-Based Outlier Detection and a Nested Loop Method

A representative method of proximity-based outlier detection uses the concept of **distance-based outliers**. For a set, D, of data objects to be analyzed, a user can specify a distance threshold, r, to define a reasonable neighborhood of an object. For each object, $\boldsymbol{o}$, we can examine the number of other objects in the r-neighborhood of $\boldsymbol{o}$. If most of the objects in D are far from $\boldsymbol{o}$, that is, not in the r-neighborhood of $\boldsymbol{o}$, then $\boldsymbol{o}$ can be regarded as an outlier.

Formally, let r ($r \geq 0$) be a *distance threshold* and π ($0 < \pi \leq 1$) be a fraction threshold. An object, $\boldsymbol{o}$, is a $DB(r,\pi)$**-outlier** if

$$\frac{\|\{\boldsymbol{o}' | dist(\boldsymbol{o},\boldsymbol{o}') \leq r\}\|}{\|D\|} \leq \pi, \tag{12.10}$$

where $dist(\cdot,\cdot)$ is a distance measure.

Equivalently, we can determine whether an object, $\boldsymbol{o}$, is a $DB(r,\pi)$-outlier by checking the distance between $\boldsymbol{o}$ and its k-nearest neighbor, $\boldsymbol{o}_k$, where $k = \lceil \pi \|D\| \rceil$. Object $\boldsymbol{o}$ is an outlier if $dist(\boldsymbol{o},\boldsymbol{o}_k) > r$, because in such a case, there are fewer than k objects except for $\boldsymbol{o}$ that are in the r-neighborhood of $\boldsymbol{o}$.

"How can we compute $DB(r,\pi)$-outliers?" A straightforward approach is to use nested loops to check the r-neighborhood for every object, as shown in Figure 12.6. For any object, $\boldsymbol{o}_i$ ($1 \leq i \leq n$), we calculate the distance between $\boldsymbol{o}_i$ and the other object, and count the number of other objects in the r-neighborhood of $\boldsymbol{o}_i$. Once we find $\pi \cdot n$ other

Algorithm: Distance-based outlier detection.

Input:

- a set of objects $D = \{\boldsymbol{o}_1, \ldots, \boldsymbol{o}_n\}$, threshold r ($r > 0$) and π ($0 < \pi \leq 1$);

Output: $DB(r,\pi)$ outliers in D.

Method:

```
for $i = 1$ to $n$ do
   $count \leftarrow 0$
   for $j = 1$ to $n$ do
      if $i \neq j$ and $dist(\boldsymbol{o}_i, \boldsymbol{o}_j) \leq r$ then
         $count \leftarrow count + 1$
         if $count \geq \pi \cdot n$ then
            exit {$\boldsymbol{o}_i$ cannot be a $DB(r,\pi)$ outlier}
         endif
      endif
   endfor
   print $\boldsymbol{o}_i$ {$\boldsymbol{o}_i$ is a $DB(r,\pi)$ outlier according to (Eq. 12.10)}
endfor;
```

Figure 12.6 Nested loop algorithm for $DB(r,\pi)$-outlier detection.

objects within a distance r from $\boldsymbol{o}_i$, the inner loop can be terminated because $\boldsymbol{o}_i$ already violates (Eq. 12.10), and thus is not a $DB(r,\pi)$-outlier. On the other hand, if the inner loop completes for $\boldsymbol{o}_i$, this means that $\boldsymbol{o}_i$ has less than $\pi \cdot n$ neighbors in a radius of r, and thus is a $DB(r,\pi)$-outlier.

The straightforward nested loop approach takes $O(n^2)$ time. Surprisingly, the actual CPU runtime is often linear with respect to the data set size. For most nonoutlier objects, the inner loop terminates early when the number of outliers in the data set is small, which should be the case most of the time. Correspondingly, only a small fraction of the data set is examined.

When mining large data sets where the complete set of objects cannot be held in main memory, the nested loop approach is still costly. Suppose the main memory has m pages for the mining. Instead of conducting the inner loop object by object, in such a case, the outer loop uses $m-1$ pages to hold as many objects as possible and uses the remaining one page to run the inner loop. The inner loop cannot stop until all objects in the $m-1$ pages are identified as not being outliers, which is very unlikely to happen. Correspondingly, it is likely that the algorithm has to incur $O((\frac{n}{b})^2)$ input/output (I/O) cost, where b is the number of objects that can be held in one page.

The major cost in the nested loop method comes from two aspects. First, to check whether an object is an outlier, the nested loop method tests the object against the whole data set. To improve, we need to explore how to determine the outlierness of an object from the neighbors that are close to the object. Second, the nested loop method checks objects one by one. To improve, we should try to group objects according to their proximity, and check the outlierness of objects group by group most of the time. Section 12.4.2 introduces how to implement the preceding ideas.

12.4.2 A Grid-Based Method

CELL is a grid-based method for distance-based outlier detection. In this method, the data space is partitioned into a multidimensional grid, where each cell is a hypercube that has a diagonal of length $\frac{r}{2}$, where r is a distance threshold parameter. In other words, if there are l dimensions, the length of each edge of a cell is $\frac{r}{2\sqrt{l}}$.

Consider a 2-D data set, for example. Figure 12.7 shows part of the grid. The length of each edge of a cell is $\frac{r}{2\sqrt{2}}$.

Consider the cell C in Figure 12.7. The neighboring cells of C can be divided into two groups. The cells immediately next to C constitute the *level-1* cells (labeled “1” in the figure), and the cells one or two cells away from C in any direction constitute the *level-2* cells (labeled “2” in the figure). The two levels of cells have the following properties:

- **Level-1 cell property**: Given any possible point, $\boldsymbol{x}$ of C, and any possible point, $\boldsymbol{y}$, in a level-1 cell, then $dist(\boldsymbol{x},\boldsymbol{y}) \leq r$.
- **Level-2 cell property**: Given any possible point, $\boldsymbol{x}$ of C, and any point, $\boldsymbol{y}$, such that $dist(\boldsymbol{x},\boldsymbol{y}) \geq r$, then $\boldsymbol{y}$ is in a level-2 cell.

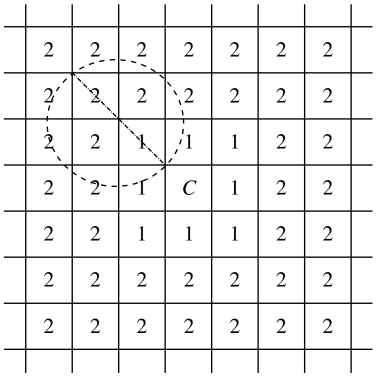


Figure 12.7 Grids in the CELL method.

Let a be the number of objects in cell C, b_1 be the total number of objects in the level-1 cells, and b_2 be the total number of objects in the level-2 cells. We can apply the following rules.

- **Level-1 cell pruning rule**: Based on the level-1 cell property, if $a + b_1 > \lceil \pi n \rceil$, then every object $\boldsymbol{o}$ in C is not a $DB(r, \pi)$-outlier because all those objects in C and the level-1 cells are in the r-neighborhood of $\boldsymbol{o}$, and there are at least $\lceil \pi n \rceil$ such neighbors.
- **Level-2 cell pruning rule**: Based on the level-2 cell property, if $a + b_1 + b_2 < \lceil \pi n \rceil + 1$, then all objects in C are $DB(r, \pi)$-outliers because each of their r-neighborhoods has less than $\lceil \pi n \rceil$ other objects.

Using the preceding two rules, the CELL method organizes objects into groups using a grid—all objects in a cell form a group. For groups satisfying one of the two rules, we can determine that either all objects in a cell are outliers or nonoutliers, and thus do not need to check those objects one by one. Moreover, to apply the two rules, we need only check a limited number of cells close to a target cell instead of the whole data set.

Using the previous two rules, many objects can be determined as being either nonoutliers or outliers. We only need to check the objects that cannot be pruned using the two rules. Even for such an object, $\boldsymbol{o}$, we need only compute the distance between $\boldsymbol{o}$ and the objects in the level-2 cells with respect to $\boldsymbol{o}$. This is because all objects in the level-1 cells have a distance of at most r to $\boldsymbol{o}$, and all objects not in a level-1 or level-2 cell must have a distance of more than r from $\boldsymbol{o}$, and thus cannot be in the r-neighborhood of $\boldsymbol{o}$.

When the data set is very large so that most of the data are stored on disk, the CELL method may incur many random accesses to disk, which is costly. An alternative method was proposed, which uses a very small amount of main memory (around 1% of the data set) to mine all outliers by scanning the data set three times. First, a sample, S, is created of the given data set, D, using sampling by replacement. Each object in S is considered the centroid of a partition. The objects in D are assigned to the partitions based on distance. The preceding steps are completed in one scan of D. Candidate outliers are identified in a second scan of D. After a third scan, all $DB(r,\pi)$-outliers have been found.

12.4.3 Density-Based Outlier Detection

Distance-based outliers, such as $DB(r,\pi)$-outliers, are just one type of outlier. Specifically, distance-based outlier detection takes a global view of the data set. Such outliers can be regarded as "global outliers" for two reasons:

- A $DB(r,\pi)$-outlier, for example, is far (as quantified by parameter r) from at least $(1-\pi) \times 100\%$ of the objects in the data set. In other words, an outlier as such is remote from the majority of the data.
- To detect distance-based outliers, we need two global parameters, r and π, which are applied to every outlier object.

Many real-world data sets demonstrate a more complex structure, where objects may be considered outliers with respect to their local neighborhoods, rather than with respect to the global data distribution. Let's look at an example.

Example 12.14 **Local proximity-based outliers.** Consider the data points in Figure 12.8. There are two clusters: C_1 is dense, and C_2 is sparse. Object $\boldsymbol{o}_3$ can be detected as a distance-based outlier because it is far from the majority of the data set.

Now, let's consider objects $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$. Are they outliers? On the one hand, the distance from $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$ to the objects in the dense cluster, C_1, is smaller than the average distance between an object in cluster C_2 and its nearest neighbor. Thus, $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$ are not distance-based outliers. In fact, if we were to categorize $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$ as $DB(r,\pi)$-outliers, we would have to classify all the objects in clusters C_2 as $DB(r,\pi)$-outliers.

On the other hand, $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$ can be identified as outliers when they are considered locally with respect to cluster C_1 because $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$ deviate significantly from the objects in C_1. Moreover, $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$ are also far from the objects in C_2.

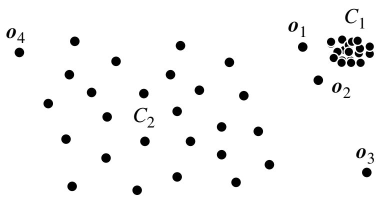


Figure 12.8 Global outliers and local outliers.

To summarize, distance-based outlier detection methods cannot capture local outliers like $\boldsymbol{o}_1$ and $\boldsymbol{o}_2$. Note that the distance between object $\boldsymbol{o}_4$ and its nearest neighbors is much greater than the distance between $\boldsymbol{o}_1$ and its nearest neighbors. However, because $\boldsymbol{o}_4$ is local to cluster C_2 (which is sparse), $\boldsymbol{o}_4$ is not considered a local outlier. ■

"How can we formulate the local outliers as illustrated in Example 12.14?" The critical idea here is that we need to compare the density around an object with the density around its local neighbors. The basic assumption of density-based outlier detection methods is that the density around a nonoutlier object is similar to the density around its neighbors, while the density around an outlier object is significantly different from the density around its neighbors.

Based on the preceding, density-based outlier detection methods use the relative density of an object against its neighbors to indicate the degree to which an object is an outlier.

Now, let's consider how to measure the *relative density* of an object, $\boldsymbol{o}$, given a set of objects, D. The *k-distance* of $\boldsymbol{o}$, denoted by $dist_k(\boldsymbol{o})$, is the distance, $dist(\boldsymbol{o}, \boldsymbol{p})$, between $\boldsymbol{o}$ and another object, $\boldsymbol{p} \in D$, such that

- There are at least k objects $\boldsymbol{o}' \in D - \{\boldsymbol{o}\}$ such that $dist(\boldsymbol{o}, \boldsymbol{o}') \leq dist(\boldsymbol{o}, \boldsymbol{p})$.
- There are at most $k - 1$ objects $\boldsymbol{o}'' \in D - \{\boldsymbol{o}\}$ such that $dist(\boldsymbol{o}, \boldsymbol{o}'') < dist(\boldsymbol{o}, \boldsymbol{p})$.

In other words, $dist_k(\boldsymbol{o})$ is the distance between $\boldsymbol{o}$ and its k-nearest neighbor. Consequently, the *k-distance neighborhood* of $\boldsymbol{o}$ contains all objects of which the distance to $\boldsymbol{o}$ is not greater than $dist_k(\boldsymbol{o})$, the k-distance of $\boldsymbol{o}$, denoted by

$$N_k(\boldsymbol{o}) = \{\boldsymbol{o}' | \boldsymbol{o}' \in D, dist(\boldsymbol{o}, \boldsymbol{o}') \leq dist_k(\boldsymbol{o})\}. \tag{12.11}$$

Note that $N_k(\boldsymbol{o})$ may contain more than k objects because multiple objects may each be the same distance away from $\boldsymbol{o}$.

We can use the average distance from the objects in $N_k(\boldsymbol{o})$ to $\boldsymbol{o}$ as the measure of the local density of $\boldsymbol{o}$. However, such a straightforward measure has a problem: If $\boldsymbol{o}$ has very close neighbors $\boldsymbol{o}'$ such that $dist(\boldsymbol{o}, \boldsymbol{o}')$ is very small, the statistical fluctuations of the distance measure can be undesirably high. To overcome this problem, we can switch to the following reachability distance measure by adding a smoothing effect.

For two objects, $\boldsymbol{o}$ and $\boldsymbol{o}'$, the *reachability distance* from $\boldsymbol{o}'$ to $\boldsymbol{o}$ is $dist(\boldsymbol{o} \leftarrow \boldsymbol{o}')$ if $dist(\boldsymbol{o}, \boldsymbol{o}') > dist_k(\boldsymbol{o})$, and $dist_k(\boldsymbol{o})$ otherwise. That is,

$$reachdist_k(\boldsymbol{o} \leftarrow \boldsymbol{o}') = \max\{dist_k(\boldsymbol{o}), dist(\boldsymbol{o}, \boldsymbol{o}')\}. \tag{12.12}$$

Here, k is a user-specified parameter that controls the smoothing effect. Essentially, k specifies the minimum neighborhood to be examined to determine the local density of an object. Importantly, reachability distance is not symmetric, that is, in general, $reachdist_k(\boldsymbol{o} \leftarrow \boldsymbol{o}') \neq reachdist_k(\boldsymbol{o}' \leftarrow \boldsymbol{o})$.

Now, we can define the *local reachability density* of an object, $\boldsymbol{o}$, as

$$lrd_k(\boldsymbol{o}) = \frac{\|N_k(\boldsymbol{o})\|}{\sum_{\boldsymbol{o}' \in N_k(\boldsymbol{o})} reachdist_k(\boldsymbol{o}' \leftarrow \boldsymbol{o})}. \tag{12.13}$$

There is a critical difference between the density measure here for outlier detection and that in density-based clustering (Section 12.5). In density-based clustering, to determine whether an object can be considered a core object in a density-based cluster, we use two parameters: a radius parameter, r, to specify the range of the neighborhood, and the minimum number of points in the r-neighborhood. Both parameters are global and are applied to every object. In contrast, as motivated by the observation that relative density is the key to finding local outliers, we use the parameter k to quantify the neighborhood and do not need to specify the minimum number of objects in the neighborhood as a requirement of density. We instead calculate the local reachability density for an object and compare it with that of its neighbors to quantify the degree to which the object is considered an outlier.

Specifically, we define the *local outlier factor* of an object $\boldsymbol{o}$ as

$$LOF_k(\boldsymbol{o}) = \frac{\sum_{\boldsymbol{o}' \in N_k(\boldsymbol{o})} \frac{lrd_k(\boldsymbol{o}')}{lrd_k(\boldsymbol{o})}}{\|N_k(\boldsymbol{o})\|} = \sum_{\boldsymbol{o}' \in N_k(\boldsymbol{o})} lrd_k(\boldsymbol{o}') \cdot \sum_{\boldsymbol{o}' \in N_k(\boldsymbol{o})} reachdist_k(\boldsymbol{o}' \leftarrow \boldsymbol{o}). \tag{12.14}$$

In other words, the local outlier factor is the average of the ratio of the local reachability density of $\boldsymbol{o}$ and those of $\boldsymbol{o}$'s k-nearest neighbors. The lower the local reachability density of $\boldsymbol{o}$ (i.e., the smaller the item $\sum_{\boldsymbol{o}' \in N_k(\boldsymbol{o})} reachdist_k(\boldsymbol{o}' \leftarrow \boldsymbol{o})$) and the higher the local reachability densities of the k-nearest neighbors of $\boldsymbol{o}$, the higher the LOF value is. This exactly captures a local outlier of which the local density is relatively low compared to the local densities of its k-nearest neighbors.

The local outlier factor has some nice properties. First, for an object deep within a consistent cluster, such as the points in the center of cluster C_2 in Figure 12.8, the local outlier factor is close to 1. This property ensures that objects inside clusters, no matter whether the cluster is dense or sparse, will not be mislabeled as outliers.

Second, for an object $\boldsymbol{o}$, the meaning of $LOF(\boldsymbol{o})$ is easy to understand. Consider the objects in Figure 12.9, for example. For object $\boldsymbol{o}$, let

$$direct_{min}(\boldsymbol{o}) = \min\{reachdist_k(\boldsymbol{o}' \leftarrow \boldsymbol{o}) | \boldsymbol{o}' \in N_k(\boldsymbol{o})\} \tag{12.15}$$

be the minimum reachability distance from $\boldsymbol{o}$ to its k-nearest neighbors. Similarly, we can define

$$direct_{max}(\boldsymbol{o}) = \max\{reachdist_k(\boldsymbol{o}' \leftarrow \boldsymbol{o}) | \boldsymbol{o}' \in N_k(\boldsymbol{o})\}. \tag{12.16}$$

We also consider the neighbors of $\boldsymbol{o}$'s k-nearest neighbors. Let

$$indirect_{min}(\boldsymbol{o}) = \min\{reachdist_k(\boldsymbol{o}'' \leftarrow \boldsymbol{o}') | \boldsymbol{o}' \in N_k(\boldsymbol{o}) \text{ and } \boldsymbol{o}'' \in N_k(\boldsymbol{o}')\} \tag{12.17}$$

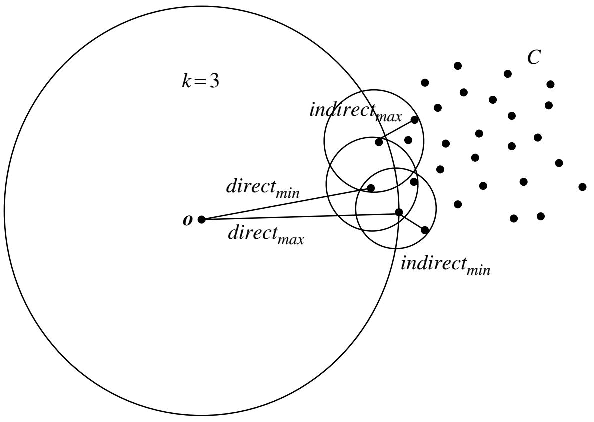


Figure 12.9 A property of $LOF(\boldsymbol{o})$.

and

$$indirect_{max}(\boldsymbol{o}) = \max\{reachdist_k(\boldsymbol{o}'' \leftarrow \boldsymbol{o}') | \boldsymbol{o}' \in N_k(\boldsymbol{o}) \text{ and } \boldsymbol{o}'' \in N_k(\boldsymbol{o}')\}. \quad (12.18)$$

Then, it can be shown that $LOF(\boldsymbol{o})$ is bounded as

$$\frac{direct_{min}(\boldsymbol{o})}{indirect_{max}(\boldsymbol{o})} \leq LOF(\boldsymbol{o}) \leq \frac{direct_{max}(\boldsymbol{o})}{indirect_{min}(\boldsymbol{o})}. \quad (12.19)$$

This result clearly shows that LOF captures the relative density of an object.

12.5 Clustering-Based Approaches

The notion of outliers is highly related to that of clusters. Clustering-based approaches detect outliers by examining the relationship between objects and clusters. Intuitively, an outlier is an object that belongs to a small and remote cluster, or does not belong to any cluster.

This leads to three general approaches to clustering-based outlier detection. Consider an object.

- Does the object belong to any cluster? If not, then it is identified as an outlier.
- Is there a large distance between the object and the cluster to which it is closest? If yes, it is an outlier.
- Is the object part of a small or sparse cluster? If yes, then all the objects in that cluster are outliers.

Let's look at examples of each of these approaches.

Example 12.15 **Detecting outliers as objects that do not belong to any cluster.** Gregarious animals (e.g., goats and deer) live and move in flocks. Using outlier detection, we can identify outliers as animals that are not part of a flock. Such animals may be either lost or wounded.

In Figure 12.10, each point represents an animal living in a group. Using a density-based clustering method, such as DBSCAN, we note that the black points belong to clusters. The white point, ***a***, does not belong to any cluster, and thus is declared an outlier. ■

The second approach to clustering-based outlier detection considers the distance between an object and the cluster to which it is closest. If the distance is large, then the object is likely an outlier with respect to the cluster. Thus, this approach detects individual outliers with respect to clusters.

Example 12.16 **Clustering-based outlier detection using distance to the closest cluster.** Using the k-means clustering method, we can partition the data points shown in Figure 12.11 into three clusters, as shown using different symbols. The center of each cluster is marked with a $+$.

For each object, $\boldsymbol{o}$, we can assign an outlier score to the object according to the distance between the object and the center that is closest to the object. Suppose the closest center to $\boldsymbol{o}$ is $\boldsymbol{c}_o$; then the distance between $\boldsymbol{o}$ and $\boldsymbol{c}_o$ is $dist(\boldsymbol{o}, \boldsymbol{c}_o)$, and the average

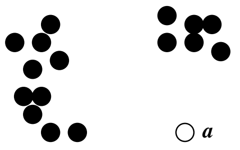


Figure 12.10 Object ***a*** is an outlier because it does not belong to any cluster.

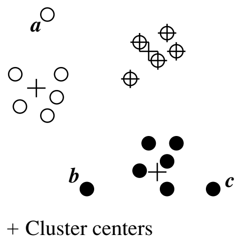


Figure 12.11 Outliers $(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})$ are far from the clusters to which they are closest (with respect to the cluster centers).

distance between $\boldsymbol{c}_o$ and the objects assigned to $\boldsymbol{o}$ is $l_{\boldsymbol{c}_o}$. The ratio $\frac{dist(\boldsymbol{o},\boldsymbol{c}_o)}{l_{\boldsymbol{c}_o}}$ measures how $dist(\boldsymbol{o}, \boldsymbol{c}_o)$ stands out from the average. The larger the ratio, the farther away $\boldsymbol{o}$ is relative from the center, and the more likely $\boldsymbol{o}$ is an outlier. In Figure 12.11, points $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ are relatively far away from their corresponding centers, and thus are suspected of being outliers. ■

This approach can also be used for intrusion detection, as described in Example 12.17.

Example 12.17 **Intrusion detection by clustering-based outlier detection.** A bootstrap method was developed to detect intrusions in TCP connection data by considering the similarity between data points and the clusters in a training data set. The method consists of three steps.

1. A training data set is used to find patterns of normal data. Specifically, the TCP connection data are segmented according to, say, dates. Frequent itemsets are found in each segment. The frequent itemsets that are in a majority of the segments are considered patterns of normal data and are referred to as "base connections."
2. Connections in the training data that contain base connections are treated as attack-free. Such connections are clustered into groups.
3. The data points in the original data set are compared with the clusters mined in step 2. Any point that is deemed an outlier with respect to the clusters is declared as a possible attack.

■

Note that each of the approaches we have seen so far detects only individual objects as outliers because they compare objects one at a time against clusters in the data set. However, in a large data set, some outliers may be similar and form a small cluster. In intrusion detection, for example, hackers who use similar tactics to attack a system may form a cluster. The approaches discussed so far may be deceived by such outliers.

To overcome this problem, a third approach to cluster-based outlier detection identifies small or sparse clusters and declares the objects in those clusters to be outliers as well. An example of this approach is the *FindCBLOF* algorithm, which works as follows.

1. Find clusters in a data set, and sort them according to decreasing size. The algorithm assumes that most of the data points are not outliers. It uses a parameter α $(0 \leq \alpha \leq 1)$ to distinguish large from small clusters. Any cluster that contains at least a percentage α (e.g., $\alpha = 90\%$) of the data set is considered a "large cluster." The remaining clusters are referred to as "small clusters."
2. To each data point, assign a *cluster-based local outlier factor* (CBLOF). For a point belonging to a large cluster, its CBLOF is the product of the cluster's size and the similarity between the point and the cluster. For a point belonging to a small cluster, its CBLOF is calculated as the product of the size of the small cluster and the similarity between the point and the closest large cluster.

CBLOF defines the similarity between a point and a cluster in a statistical way that represents the probability that the point belongs to the cluster. The larger the value, the more similar the point and the cluster are. The CBLOF score can detect outlier points that are far from any clusters. In addition, small clusters that are far from any large cluster are considered to consist of outliers. The points with the lowest CBLOF scores are suspected outliers.

Example 12.18 **Detecting outliers in small clusters.** The data points in Figure 12.12 form three clusters: large clusters, C_1 and C_2, and a small cluster, C_3. Object $\boldsymbol{o}$ does not belong to any cluster.

Using CBLOF, *FindCBLOF* can identify $\boldsymbol{o}$ as well as the points in cluster C_3 as outliers. For $\boldsymbol{o}$, the closest large cluster is C_1. The CBLOF is simply the similarity between $\boldsymbol{o}$ and C_1, which is small. For the points in C_3, the closest large cluster is C_2. Although there are three points in cluster C_3, the similarity between those points and cluster C_2 is low, and $|C_3| = 3$ is small; thus, the CBLOF scores of points in C_3 are small. ■

Clustering-based approaches may incur high computational costs if they have to find clusters before detecting outliers. Several techniques have been developed for improved efficiency. For example, **fixed-width clustering** is a linear-time technique that is used in some outlier detection methods. The idea is simple yet efficient. A point is assigned to a cluster if the center of the cluster is within a predefined distance threshold from the point. If a point cannot be assigned to any existing cluster, a new cluster is created. The distance threshold may be learned from the training data under certain conditions.

Clustering-based outlier detection methods have the following advantages. First, they can detect outliers without requiring any labeled data, that is, in an unsupervised way. They work for many data types. Clusters can be regarded as summaries of the data. Once the clusters are obtained, clustering-based methods need only compare any object against the clusters to determine whether the object is an outlier. This process is typically fast because the number of clusters is usually small compared to the total number of objects.

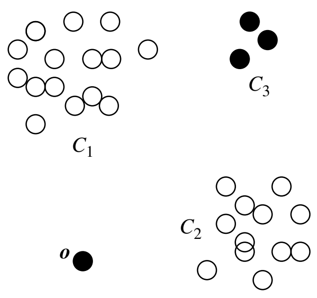


Figure 12.12 Outliers in small clusters.

A weakness of clustering-based outlier detection is its effectiveness, which depends highly on the clustering method used. Such methods may not be optimized for outlier detection. Clustering methods are often costly for large data sets, which can serve as a bottleneck.

12.6 Classification-Based Approaches

Outlier detection can be treated as a classification problem if a training data set with class labels is available. The general idea of classification-based outlier detection methods is to train a classification model that can distinguish normal data from outliers.

Consider a training set that contains samples labeled as "normal" and others labeled as "outlier." A classifier can then be constructed based on the training set. Any classification method can be used (Chapters 8 and 9). This kind of brute-force approach, however, does not work well for outlier detection because the training set is typically heavily biased. That is, the number of normal samples likely far exceeds the number of outlier samples. This imbalance, where the number of outlier samples may be insufficient, can prevent us from building an accurate classifier. Consider intrusion detection in a system, for example. Because most system accesses are normal, it is easy to obtain a good representation of the normal events. However, it is infeasible to enumerate all potential intrusions, as new and unexpected attempts occur from time to time. Hence, we are left with an insufficient representation of the outlier (or intrusion) samples.

To overcome this challenge, classification-based outlier detection methods often use a *one-class model*. That is, a classifier is built to describe only the normal class. Any samples that do not belong to the normal class are regarded as outliers.

Example 12.19 Outlier detection using a one-class model. Consider the training set shown in Figure 12.13, where white points are samples labeled as "normal" and black points are samples labeled as "outlier." To build a model for outlier detection, we can learn the decision boundary of the normal class using classification methods such as SVM (Chapter 9), as illustrated. Given a new object, if the object is within the decision boundary of the normal class, it is treated as a normal case. If the object is outside the decision boundary, it is declared an outlier.

An advantage of using only the model of the normal class to detect outliers is that the model can detect new outliers that may not appear close to any outlier objects in the training set. This occurs as long as such new outliers fall outside the decision boundary of the normal class. ■

The idea of using the decision boundary of the normal class can be extended to handle situations where the normal objects may belong to multiple classes such as in fuzzy clustering (Chapter 11). For example, *AllElectronics* accepts returned items. Customers can return items for a number of reasons (corresponding to class categories) such as "product design defects" and "product damaged during shipment." Each such

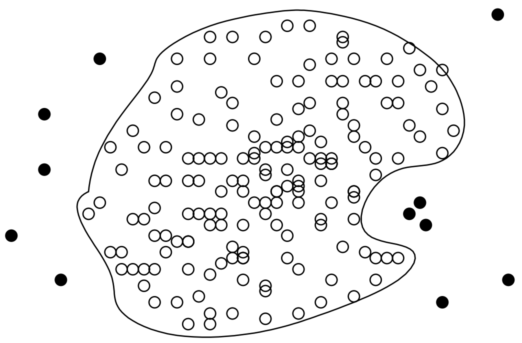


Figure 12.13 Learning a model for the normal class.

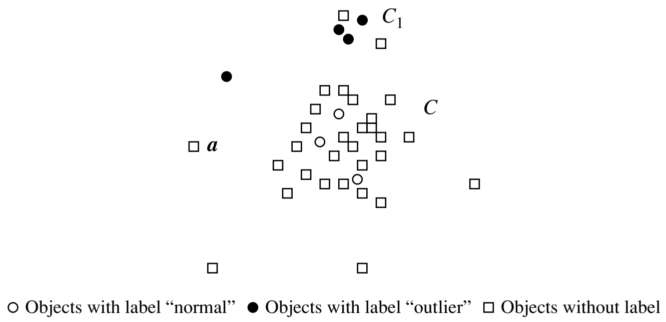

C_1
C
a
○ Objects with label "normal" ● Objects with label "outlier" □ Objects without label

Figure 12.14 Detecting outliers by semi-supervised learning.

class is regarded as normal. To detect outlier cases, *AllElectronics* can learn a model for each normal class. To determine whether a case is an outlier, we can run each model on the case. If the case does not fit any of the models, then it is declared an outlier.

Classification-based methods and clustering-based methods can be combined to detect outliers in a semi-supervised learning way.

Example 12.20 **Outlier detection by semi-supervised learning.** Consider Figure 12.14, where objects are labeled as either "normal" or "outlier," or have no label at all. Using a clustering-based approach, we find a large cluster, C, and a small cluster, C_1. Because some objects in C carry the label "normal," we can treat all objects in this cluster (including those without labels) as normal objects. We use the one-class model of this cluster to identify normal objects in outlier detection. Similarly, because some objects in cluster C_1 carry the label "outlier," we declare all objects in C_1 as outliers. Any object that does not fall into the model for C (e.g., $\boldsymbol{a}$) is considered an outlier as well. ■

Classification-based methods can incorporate human domain knowledge into the detection process by learning from the labeled samples. Once the classification model is constructed, the outlier detection process is fast. It only needs to compare the objects to be examined against the model learned from the training data. The quality of classification-based methods heavily depends on the availability and quality of the training set. In many applications, it is difficult to obtain representative and high-quality training data, which limits the applicability of classification-based methods.

12.7 Mining Contextual and Collective Outliers

An object in a given data set is a **contextual outlier** (or *conditional outlier*) if it deviates significantly with respect to a specific context of the object (Section 12.1). The context is defined using **contextual attributes**. These depend heavily on the application, and are often provided by users as part of the contextual outlier detection task. Contextual attributes can include spatial attributes, time, network locations, and sophisticated structured attributes. In addition, **behavioral attributes** define characteristics of the object, and are used to evaluate whether the object is an outlier in the context to which it belongs.

Example 12.21 **Contextual outliers.** To determine whether the temperature of a location is exceptional (i.e., an outlier), the attributes specifying information about the location can serve as contextual attributes. These attributes may be spatial attributes (e.g., longitude and latitude) or location attributes in a graph or network. The attribute *time* can also be used. In customer-relationship management, whether a customer is an outlier may depend on other customers with similar profiles. Here, the attributes defining customer profiles provide the context for outlier detection. ■

In comparison to outlier detection in general, identifying contextual outliers requires analyzing the corresponding contextual information. Contextual outlier detection methods can be divided into two categories according to whether the contexts can be clearly identified.

12.7.1 Transforming Contextual Outlier Detection to Conventional Outlier Detection

This category of methods is for situations where the contexts can be clearly identified. The idea is to transform the contextual outlier detection problem into a typical outlier detection problem. Specifically, for a given data object, we can evaluate whether the object is an outlier in two steps. In the first step, we identify the context of the object using the contextual attributes. In the second step, we calculate the outlier score for the object in the context using a conventional outlier detection method.

Example 12.22 **Contextual outlier detection when the context can be clearly identified.** In customer-relationship management, we can detect outlier customers in the context of customer groups. Suppose *AllElectronics* maintains customer information on four attributes, namely *age_group* (i.e., under 25, 25-45, 45-65, and over 65), *postal_code*, *number_of_transactions_per_year*, and *annual_total_transaction_amount*. The attributes *age_group* and *postal_code* serve as contextual attributes, and the attributes *number_of_transactions_per_year* and *annual_total_transaction_amount* are behavioral attributes. ■

To detect contextual outliers in this setting, for a customer, ***c***, we can first locate the context of ***c*** using the attributes *age_group* and *postal_code*. We can then compare ***c*** with the other customers in the same group, and use a conventional outlier detection method, such as some of the ones discussed earlier, to determine whether ***c*** is an outlier.

Contexts may be specified at different levels of granularity. Suppose *AllElectronics* maintains customer information at a more detailed level for the attributes *age*, *postal_code*, *number_of_transactions_per_year*, and *annual_total_transaction_amount*. We can still group customers on *age* and *postal_code*, and then mine outliers in each group. What if the number of customers falling into a group is very small or even zero? For a customer, ***c***, if the corresponding context contains very few or even no other customers, the evaluation of whether ***c*** is an outlier using the exact context is unreliable or even impossible.

To overcome this challenge, we can assume that customers of similar age and who live within the same area should have similar normal behavior. This assumption can help to generalize contexts and makes for more effective outlier detection. For example, using a set of training data, we may learn a mixture model, U, of the data on the contextual attributes, and another mixture model, V, of the data on the behavior attributes. A mapping $p(V_i|U_j)$ is also learned to capture the probability that a data object $\boldsymbol{o}$ belonging to cluster U_j on the contextual attributes is generated by cluster V_i on the behavior attributes. The outlier score can then be calculated as

$$S(\boldsymbol{o}) = \sum_{U_j} p(\boldsymbol{o} \in U_j) \sum_{V_i} p(\boldsymbol{o} \in V_i) p(V_i|U_j). \tag{12.20}$$

Thus, the contextual outlier problem is transformed into outlier detection using mixture models.

12.7.2 Modeling Normal Behavior with Respect to Contexts

In some applications, it is inconvenient or infeasible to clearly partition the data into contexts. For example, consider the situation where the online store of *AllElectronics* records customer browsing behavior in a search log. For each customer, the data log contains the sequence of products searched for and browsed by the customer. *AllElectronics* is interested in contextual outlier behavior, such as if a customer suddenly purchased a product that is unrelated to those she recently browsed. However, in this application, contexts cannot be easily specified because it is unclear how many products browsed earlier should be considered as the context, and this number will likely differ for each product.

This second category of contextual outlier detection methods models the normal behavior with respect to contexts. Using a training data set, such a method trains a model that predicts the expected behavior attribute values with respect to the contextual attribute values. To determine whether a data object is a contextual outlier, we can then apply the model to the contextual attributes of the object. If the behavior attribute values of the object significantly deviate from the values predicted by the model, then the object can be declared a contextual outlier.

By using a prediction model that links the contexts and behavior, these methods avoid the explicit identification of specific contexts. A number of classification and prediction techniques can be used to build such models such as regression, Markov models, and finite state automaton. Interested readers are referred to Chapters 8 and 9 on classification and the bibliographic notes for further details (Section 12.11).

In summary, contextual outlier detection enhances conventional outlier detection by considering contexts, which are important in many applications. We may be able to detect outliers that cannot be detected otherwise. Consider a credit card user whose income level is low but whose expenditure patterns are similar to those of millionaires. This user can be detected as a contextual outlier if the income level is used to define context. Such a user may not be detected as an outlier without contextual information because she does share expenditure patterns with many millionaires. Considering contexts in outlier detection can also help to avoid false alarms. Without considering the context, a millionaire's purchase transaction may be falsely detected as an outlier if the majority of customers in the training set are not millionaires. This can be corrected by incorporating contextual information in outlier detection.

12.7.3 Mining Collective Outliers

A group of data objects forms a **collective outlier** if the objects as a whole deviate significantly from the entire data set, even though each individual object in the group may not be an outlier (Section 12.1). To detect collective outliers, we have to examine the *structure* of the data set, that is, the relationships between multiple data objects. This makes the problem more difficult than conventional and contextual outlier detection.

"*How can we explore the data set structure?*" This typically depends on the nature of the data. For outlier detection in temporal data (e.g., time series and sequences), we explore the structures formed by time, which occur in segments of the time series or subsequences. To detect collective outliers in spatial data, we explore local areas. Similarly, in graph and network data, we explore subgraphs. Each of these structures is inherent to its respective data type.

Contextual outlier detection and collective outlier detection are similar in that they both explore structures. In contextual outlier detection, the structures are the contexts, as specified by the contextual attributes explicitly. The critical difference in collective outlier detection is that the structures are often not explicitly defined, and have to be discovered as part of the outlier detection process.

As with contextual outlier detection, collective outlier detection methods can also be divided into two categories. The first category consists of methods that reduce the problem to conventional outlier detection. Its strategy is to identify *structure units*, treat each structure unit (e.g., a subsequence, a time-series segment, a local area, or a subgraph) as a data object, and extract features. The problem of collective outlier detection is thus transformed into outlier detection on the set of "structured objects" constructed as such using the extracted features. A structure unit, which represents a group of objects in the original data set, is a collective outlier if the structure unit deviates significantly from the expected trend in the space of the extracted features.

Example 12.23 **Collective outlier detection on graph data.** Let's see how we can detect collective outliers in *AllElectronics*' online social network of customers. Suppose we treat the social network as an unlabeled graph. We then treat each possible subgraph of the network as a structure unit. For each subgraph, S, let $|S|$ be the number of vertices in S, and $freq(S)$ be the frequency of S in the network. That is, $freq(S)$ is the number of different subgraphs in the network that are isomorphic to S. We can use these two features to detect outlier subgraphs. An *outlier subgraph* is a collective outlier that contains multiple vertices.

In general, a small subgraph (e.g., a single vertex or a pair of vertices connected by an edge) is expected to be frequent, and a large subgraph is expected to be infrequent. Using the preceding simple method, we can detect small subgraphs that are of very low frequency or large subgraphs that are surprisingly frequent. These are outlier structures in the social network. ■

Predefining the structure units for collective outlier detection can be difficult or impossible. Consequently, the second category of methods models the expected behavior of structure units directly. For example, to detect collective outliers in temporal sequences, one method is to learn a Markov model from the sequences. A subsequence can then be declared as a collective outlier if it significantly deviates from the model.

In summary, collective outlier detection is subtle due to the challenge of exploring the structures in data. The exploration typically uses heuristics, and thus may be application-dependent. The computational cost is often high due to the sophisticated mining process. While highly useful in practice, collective outlier detection remains a challenging direction that calls for further research and development.

12.8 Outlier Detection in High-Dimensional Data

In some applications, we may need to detect outliers in high-dimensional data. The dimensionality curse poses huge challenges for effective outlier detection. As the dimensionality increases, the distance between objects may be heavily dominated by noise. That is, the distance and similarity between two points in a high-dimensional space may not reflect the real relationship between the points. Consequently, conventional outlier detection methods, which mainly use proximity or density to identify outliers, deteriorate as dimensionality increases.

Ideally, outlier detection methods for high-dimensional data should meet the challenges that follow.

- **Interpretation of outliers:** They should be able to not only detect outliers, but also provide an interpretation of the outliers. Because many features (or dimensions) are involved in a high-dimensional data set, detecting outliers without providing any interpretation as to why they are outliers is not very useful. The interpretation of outliers may come from, for example, specific subspaces that manifest the outliers or an assessment regarding the "outlier-ness" of the objects. Such interpretation can help users to understand the possible meaning and significance of the outliers.
- **Data sparsity:** The methods should be capable of handling sparsity in high-dimensional spaces. The distance between objects becomes heavily dominated by noise as the dimensionality increases. Therefore, data in high-dimensional spaces are often sparse.
- **Data subspaces:** They should model outliers appropriately, for example, adaptive to the subspaces signifying the outliers and capturing the local behavior of data. Using a fixed-distance threshold against all subspaces to detect outliers is not a good idea because the distance between two objects monotonically increases as the dimensionality increases.
- **Scalability with respect to dimensionality:** As the dimensionality increases, the number of subspaces increases exponentially. An exhaustive combinatorial exploration of the search space, which contains all possible subspaces, is not a scalable choice.

Outlier detection methods for high-dimensional data can be divided into three main approaches. These include extending conventional outlier detection (Section 12.8.1), finding outliers in subspaces (Section 12.8.2), and modeling high-dimensional outliers (Section 12.8.3).

12.8.1 Extending Conventional Outlier Detection

One approach for outlier detection in high-dimensional data extends conventional outlier detection methods. It uses the conventional proximity-based models of outliers. However, to overcome the deterioration of proximity measures in high-dimensional spaces, it uses alternative measures or constructs subspaces and detects outliers there.

The **HilOut** algorithm is an example of this approach. HilOut finds distance-based outliers, but uses the ranks of distance instead of the absolute distance in outlier detection. Specifically, for each object, $\boldsymbol{o}$, HilOut finds the k-nearest neighbors of $\boldsymbol{o}$, denoted by $nn_1(\boldsymbol{o}), \ldots, nn_k(\boldsymbol{o})$, where k is an application-dependent parameter. The weight of object $\boldsymbol{o}$ is defined as

$$w(\boldsymbol{o}) = \sum_{i=1}^{k} dist(\boldsymbol{o}, nn_i(\boldsymbol{o})). \tag{12.21}$$

All objects are ranked in weight-descending order. The top-l objects in weight are output as outliers, where l is another user-specified parameter.

Computing the k-nearest neighbors for every object is costly and does not scale up when the dimensionality is high and the database is large. To address the scalability issue, HilOut employs space-filling curves to achieve an approximation algorithm, which is scalable in both running time and space with respect to database size and dimensionality.

While some methods like HilOut detect outliers in the full space despite the high dimensionality, other methods reduce the high-dimensional outlier detection problem to a lower-dimensional one by dimensionality reduction (Chapter 3). The idea is to reduce the high-dimensional space to a lower-dimensional space where normal instances can still be distinguished from outliers. If such a lower-dimensional space can be found, then conventional outlier detection methods can be applied.

To reduce dimensionality, general feature selection and extraction methods may be used or extended for outlier detection. For example, principal components analysis (PCA) can be used to extract a lower-dimensional space. Heuristically, the principal components with low variance are preferred because, on such dimensions, normal objects are likely close to each other and outliers often deviate from the majority.

By extending conventional outlier detection methods, we can reuse much of the experience gained from research in the field. These new methods, however, are limited. First, they cannot detect outliers with respect to subspaces and thus have limited interpretability. Second, dimensionality reduction is feasible only if there exists a lower-dimensional space where normal objects and outliers are well separated. This assumption may not hold true.

12.8.2 Finding Outliers in Subspaces

Another approach for outlier detection in high-dimensional data is to search for outliers in various subspaces. A unique advantage is that, if an object is found to be an outlier in a subspace of much lower dimensionality, the subspace provides critical information for interpreting *why* and *to what extent* the object is an outlier. This insight is highly valuable in applications with high-dimensional data due to the overwhelming number of dimensions.

Example 12.24 **Outliers in subspaces.** As a customer-relationship manager at *AllElectronics*, you are interested in finding outlier customers. *AllElectronics* maintains an extensive customer information database, which contains many attributes and the transaction history of customers. The database is high dimensional.

Suppose you find that a customer, Alice, is an outlier in a lower-dimensional subspace that contains the dimensions *average_transaction_amount* and *purchase_frequency*, such that her average transaction amount is substantially larger than the majority of the customers, and her purchase frequency is dramatically lower. The subspace itself speaks for why and to what extent Alice is an outlier. Using this information, you strategically decide to approach Alice by suggesting options that could improve her purchase frequency at *AllElectronics*. ■

"How can we detect outliers in subspaces?" We use a *grid-based subspace outlier detection method* to illustrate. The major ideas are as follows. We consider projections of the data onto various subspaces. If, in a subspace, we find an area that has a density that is much lower than average, then the area may contain outliers. To find such projections, we first discretize the data into a grid in an equal-depth way. That is, each dimension is partitioned into ϕ equal-depth ranges, where each range contains a fraction, f, of the objects $\left(f = \frac{1}{\phi}\right)$. Equal-depth partitioning is used because data along different dimensions may have different localities. An equal-width partitioning of the space may not be able to reflect such differences in locality.

Next, we search for regions defined by ranges in subspaces that are significantly sparse. To quantify what we mean by "significantly sparse," let's consider a k-dimensional cube formed by k ranges on k dimensions. Suppose the data set contains n objects. If the objects are independently distributed, the expected number of objects falling into a k-dimensional region is $\left(\frac{1}{\phi}\right)^k n = f^k n$. The standard deviation of the number of points in a k-dimensional region is $\sqrt{f^k(1-f^k)n}$. Suppose a specific k-dimensional cube C has $n(C)$ objects. We can define the **sparsity coefficient** of C as

$$S(C) = \frac{n(C) - f^k n}{\sqrt{f^k(1-f^k)n}}. \tag{12.22}$$

If $S(C) < 0$, then C contains fewer objects than expected. The smaller the value of $S(C)$ (i.e., the more negative), the sparser C is and the more likely the objects in C are outliers in the subspace.

By assuming $S(C)$ follows a normal distribution, we can use normal distribution tables to determine the probabilistic significance level for an object that deviates dramatically from the average for an a priori assumption of the data following a uniform distribution. In general, the assumption of uniform distribution does not hold. However, the sparsity coefficient still provides an intuitive measure of the "outlier-ness" of a region.

To find cubes of significantly small sparsity coefficient values, a brute-force approach is to search every cube in every possible subspace. The cost of this, however, is immediately exponential. An *evolutionary search* can be conducted, which improves efficiency at the expense of accuracy. For details, please refer to the bibliographic notes (Section 12.11). The objects contained by cubes of very small sparsity coefficient values are output as outliers.

In summary, searching for outliers in subspaces is advantageous in that the outliers found tend to be better understood, owing to the context provided by the subspaces. Challenges include making the search efficient and scalable.

12.8.3 Modeling High-Dimensional Outliers

An alternative approach for outlier detection methods in high-dimensional data tries to develop new models for high-dimensional outliers directly. Such models typically avoid proximity measures and instead adopt new heuristics to detect outliers, which do not deteriorate in high-dimensional data.

Let's examine *angle-based outlier detection* (ABOD) as an example.

Example 12.25 **Angle-based outliers.** Figure 12.15 contains a set of points forming a cluster, with the exception of $\boldsymbol{c}$, which is an outlier. For each point $\boldsymbol{o}$, we examine the angle $\angle \boldsymbol{xoy}$ for every pair of points $\boldsymbol{x}, \boldsymbol{y}$ such that $\boldsymbol{x} \neq \boldsymbol{o}, \boldsymbol{y} \neq \boldsymbol{o}$. The figure shows angle $\angle \boldsymbol{dae}$ as an example.

Note that for a point in the center of a cluster (e.g., $\boldsymbol{a}$), the angles formed as such differ widely. For a point that is at the border of a cluster (e.g., $\boldsymbol{b}$), the angle variation is smaller. For a point that is an outlier (e.g., $\boldsymbol{c}$), the angle variable is substantially smaller. This observation suggests that we can use the variance of angles for a point to determine whether a point is an outlier. ■

We can combine angles and distance to model outliers. Mathematically, for each point $\boldsymbol{o}$, we use the distance-weighted angle variance as the outlier score. That is, given a set of points, D, for a point, $\boldsymbol{o} \in D$, we define the **angle-based outlier factor** (ABOF) as

$$ABOF(\boldsymbol{o}) = VAR_{x,y \in D, x \neq o, y \neq o} \frac{\langle \overrightarrow{\boldsymbol{ox}}, \overrightarrow{\boldsymbol{oy}} \rangle}{dist(\boldsymbol{o},\boldsymbol{x})^2 dist(\boldsymbol{o},\boldsymbol{y})^2}, \tag{12.23}$$

where $\langle , \rangle$ is the scalar product operator, and $dist(,)$ is a norm distance.

Clearly, the farther away a point is from clusters and the smaller the variance of the angles of a point, the smaller the ABOF. The ABOD computes the ABOF for each point, and outputs a list of the points in the data set in ABOF-ascending order.

Computing the exact ABOF for every point in a database is costly, requiring a time complexity of $O(n^3)$, where n is the number of points in the database. Obviously, this exact algorithm does not scale up for large data sets. Approximation methods have been developed to speed up the computation. The angle-based outlier detection idea has been generalized to handle arbitrary data types. For additional details, see the bibliographic notes (Section 12.11).

Developing native models for high-dimensional outliers can lead to effective methods. However, finding good heuristics for detecting high-dimensional outliers is difficult. Efficiency and scalability on large and high-dimensional data sets are major challenges.

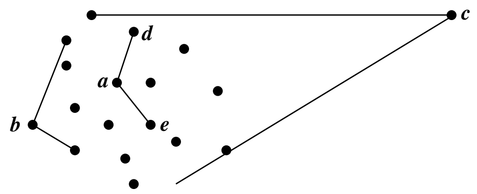


Figure 12.15 Angle-based outliers.

12.9 Summary

- Assume that a given statistical process is used to generate a set of data objects. An **outlier** is a data object that deviates significantly from the rest of the objects, as if it were generated by a different mechanism.
- **Types of outliers** include global outliers, contextual outliers, and collective outliers. An object may be more than one type of outlier.
- **Global outliers** are the simplest form of outlier and the easiest to detect. A **contextual outlier** deviates significantly with respect to a specific context of the object (e.g., a Toronto temperature value of 28°C is an outlier if it occurs in the context of winter). A subset of data objects forms a **collective outlier** if the objects as a whole deviate significantly from the entire data set, even though the individual data objects may not be outliers. Collective outlier detection requires background information to model the relationships among objects to find outlier groups.
- **Challenges** in outlier detection include finding appropriate data models, the dependence of outlier detection systems on the application involved, finding ways to distinguish outliers from noise, and providing justification for identifying outliers as such.
- Outlier detection methods can be **categorized** according to whether the sample of data for analysis is given with expert-provided labels that can be used to build an outlier detection model. In this case, the detection methods are *supervised*, *semi-supervised*, or *unsupervised*. Alternatively, outlier detection methods may be organized according to their assumptions regarding normal objects versus outliers. This categorization includes *statistical* methods, *proximity-based* methods, and *clustering-based* methods.
- **Statistical outlier detection methods** (or **model-based methods**) assume that the normal data objects follow a statistical model, where data not following the model are considered outliers. Such methods may be *parametric* (they assume that the data are generated by a parametric distribution) or *nonparametric* (they learn a model for the data, rather than assuming one a priori). Parametric methods for multivariate data may employ the Mahalanobis distance, the χ^2-statistic, or a mixture of multiple parametric models. Histograms and kernel density estimation are examples of nonparametric methods.
- **Proximity-based outlier detection methods** assume that an object is an outlier if the proximity of the object to its nearest neighbors significantly deviates from the proximity of most of the other objects to their neighbors in the same data set. *Distance-based outlier detection methods* consult the *neighborhood* of an object, defined by a given radius. An object is an outlier if its neighborhood does not have enough other points. In *density-based outlier detection methods*, an object is an outlier if its density is relatively much lower than that of its neighbors.

- **Clustering-based outlier detection methods** assume that the normal data objects belong to large and dense clusters, whereas outliers belong to small or sparse clusters, or do not belong to any clusters.
- **Classification-based outlier detection methods** often use a one-class model. That is, a classifier is built to describe only the normal class. Any samples that do not belong to the normal class are regarded as outliers.
- **Contextual outlier detection** and **collective outlier detection** explore structures in the data. In contextual outlier detection, the structures are defined as contexts using contextual attributes. In collective outlier detection, the structures are implicit and are explored as part of the mining process. To detect such outliers, one approach transforms the problem into one of conventional outlier detection. Another approach models the structures directly.
- **Outlier detection methods for high-dimensional data** can be divided into three main approaches. These include extending conventional outlier detection, finding outliers in subspaces, and modeling high-dimensional outliers.

12.10 Exercises

12.1 Give an application example where global outliers, contextual outliers, and collective outliers are all interesting. What are the attributes, and what are the contextual and behavioral attributes? How is the relationship among objects modeled in collective outlier detection?

12.2 Give an application example of where the border between normal objects and outliers is often unclear, so that the degree to which an object is an outlier has to be well estimated.

12.3 Adapt a simple semi-supervised method for outlier detection. Discuss the scenario where you have (a) only some labeled examples of normal objects, and (b) only some labeled examples of outliers.

12.4 Using an equal-depth histogram, design a way to assign an object an outlier score.

12.5 Consider the nested loop approach to mining distance-based outliers (Figure 12.6). Suppose the objects in a data set are arranged randomly, that is, each object has the same probability to appear in a position. Show that when the number of outlier objects is small with respect to the total number of objects in the whole data set, the expected number of distance calculations is linear to the number of objects.

12.6 In the density-based outlier detection method of Section 12.4.3, the definition of local reachability density has a potential problem: $lrd_k(o) = \infty$ may occur. Explain why this may occur and propose a fix to the issue.

12.7 Because clusters may form a hierarchy, outliers may belong to different granularity levels. Propose a clustering-based outlier detection method that can find outliers at different levels.

12.8 In outlier detection by semi-supervised learning, what is the advantage of using objects without labels in the training data set?

12.9 To understand why angle-based outlier detection is a heuristic method, give an example where it does not work well. Can you come up with a method to overcome this issue?

12.11 Bibliographic Notes

Hawkins [Haw80] defined outliers from a statistics angle. For surveys or tutorials on the subject of outlier and anomaly detection, see Chandola, Banerjee, and Kumar [CBK09]; Hodge and Austin [HA04]; Agyemang, Barker, and Alhajj [ABA06]; Markou and Singh [MS03a, MS03b]; Patcha and Park [PP07]; Beckman and Cook [BC83]; Ben-Gal [B-G05]; and Bakar, Mohemad, Ahmad, and Deris [BMAD06]. Song, Wu, Jermaine, et al. [SWJR-07] proposed the notion of conditional anomaly and contextual outlier detection.

Fujimaki, Yairi, and Machida [FYM05] presented an example of semi-supervised outlier detection using a set of labeled "normal" objects. For an example of semi-supervised outlier detection using labeled outliers, see Dasgupta and Majumdar [DM02].

Shewhart [She31] assumed that most objects follow a Gaussian distribution and used 3σ as the threshold for identifying outliers, where σ is the standard deviation. Boxplots are used to detect and visualize outliers in various applications such as medical data (Horn, Feng, Li, and Pesce [HFLP01]). Grubb's test was described by Grubbs [Gru69], Stefansky [Ste72], and Anscombe and Guttman [AG60]. Laurikkala, Juhola, and Kentala [LJK00] and Aggarwal and Yu [AY01] extended Grubb's test to detect multivariate outliers. Use of the χ^2-statistic to detect multivariate outliers was studied by Ye and Chen [YC01].

Agarwal [Aga06] used Gaussian mixture models to capture "normal data." Abraham and Box [AB79] assumed that outliers are generated by a normal distribution with a substantially larger variance. Eskin [Esk00] used the EM algorithm to learn mixture models for normal data and outliers.

Histogram-based outlier detection methods are popular in the application domain of intrusion detection (Eskin [Esk00] and Eskin, Arnold, Prerau, et al. [EAP$^+$02]) and fault detection (Fawcett and Provost [FP97]).

The notion of distance-based outliers was developed by Knorr and Ng [KN97]. The index-based, nested loop–based, and grid-based approaches were explored (Knorr and Ng [KN98] and Knorr, Ng, and Tucakov [KNT00]) to speed up distance-based outlier detection. Bay and Schwabacher [BS03] and Jin, Tung, and Han [JTH01] pointed out that the CPU runtime of the nested loop method is often scalable with respect to database size. Tao, Xiao, and Zhou [TXZ06] presented an algorithm that finds all distance-based outliers by scanning the database three times with fixed main memory. For larger memory size, they proposed a method that uses only one or two scans.

The notion of density-based outliers was first developed by Breunig, Kriegel, Ng, and Sander [BKNS00]. Various methods proposed with the theme of density-based outlier detection include Jin, Tung, and Han [JTH01]; Jin, Tung, Han, and Wang [JTHW06]; and Papadimitriou, Kitagawa, Gibbons, et al. [PKG-F03]. The variations differ in how they estimate density.

The bootstrap method discussed in Example 12.17 was developed by Barbara, Li, Couto, et al. [BLC$^+$03]. The FindCBOLF algorithm was given by He, Xu, and Deng [HXD03]. For the use of fixed-width clustering in outlier detection methods, see Eskin, Arnold, and Prerau, et al. [EAP$^+$02]; Mahoney and Chan [MC03]; and He, Xu, and Deng [HXD03]. Barbara, Wu, and Jajodia [BWJ01] used multiclass classification in network intrusion detection.

Song, Wu, Jermaine, et al. [SWJR07] and Fawcet and Provost [FP97] presented a method to reduce the problem of contextual outlier detection to one of conventional outlier detection. Yi, Sidiropoulos, Johnson, Jagadish, et al. [YSJJ$^+$00] used regression techniques to detect contextual outliers in co-evolving sequences. The idea in Example 12.22 for collective outlier detection on graph data is based on Noble and Cook [NC03].

The HilOut algorithm was proposed by Angiulli and Pizzuti [AP05]. Aggarwal and Yu [AY01] developed the sparsity coefficient–based subspace outlier detection method. Kriegel, Schubert, and Zimek [KSZ08] proposed angle-based outlier detection.

13 Data Mining Trends and Research Frontiers

As a young research field, data mining has made significant progress and covered a broad spectrum of applications since the 1980s. Today, data mining is used in a vast array of areas. Numerous commercial data mining systems and services are available. Many challenges, however, still remain. In this final chapter, we introduce the mining of complex data types as a prelude to further in-depth study readers may choose to do. In addition, we focus on trends and research frontiers in data mining. Section 13.1 presents an overview of methodologies for mining complex data types, which extend the concepts and tasks introduced in this book. Such mining includes mining time-series, sequential patterns, and biological sequences; graphs and networks; spatiotemporal data, including geospatial data, moving-object data, and cyber-physical system data; multimedia data; text data; web data; and data streams. Section 13.2 briefly introduces other approaches to data mining, including statistical methods, theoretical foundations, and visual and audio data mining.

In Section 13.3, you will learn more about data mining applications in business and in science, including the financial retail, and telecommunication industries, science and engineering, and recommender systems. The social impacts of data mining are discussed in Section 13.4, including ubiquitous and invisible data mining, and privacy-preserving data mining. Finally, in Section 13.5 we speculate on current and expected data mining trends that arise in response to new challenges in the field.

13.1 Mining Complex Data Types

In this section, we outline the major developments and research efforts in mining complex data types. Complex data types are summarized in Figure 13.1. Section 13.1.1 covers mining sequence data such as time-series, symbolic sequences, and biological sequences. Section 13.1.2 discusses mining graphs and social and information networks. Section 13.1.3 addresses mining other kinds of data, including spatial data, spatiotemporal data, moving-object data, cyber-physical system data, multimedia data, text data,

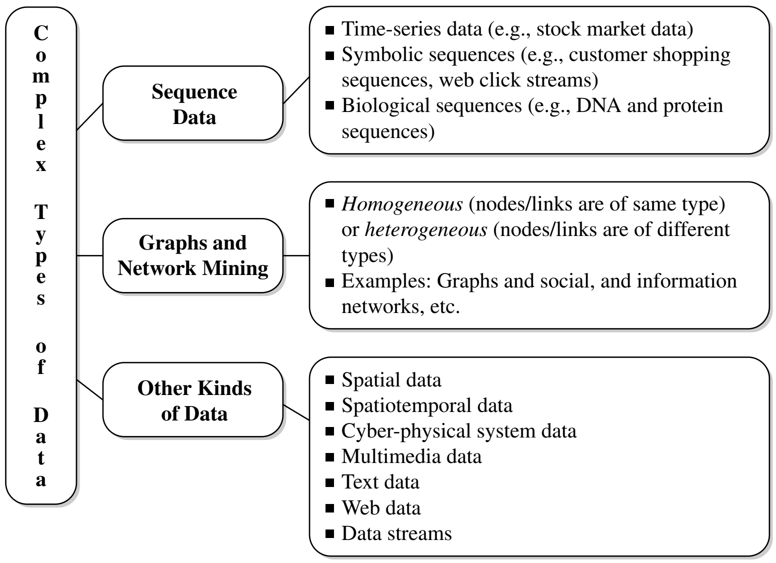

Complex Types of Data
Sequence Data
Time-series data (e.g., stock market data)
Symbolic sequences (e.g., customer shopping sequences, web click streams)
Biological sequences (e.g., DNA and protein sequences)
Graphs and Network Mining
Homogeneous (nodes/links are of same type) or heterogeneous (nodes/links are of different types)
Examples: Graphs and social, and information networks, etc.
Other Kinds of Data
Spatial data
Spatiotemporal data
Cyber-physical system data
Multimedia data
Text data
Web data
Data streams

Figure 13.1 Complex data types for mining.

web data, and data streams. Due to the broad scope of these themes, this section presents only a high-level overview; these topics are not discussed in-depth in this book.

13.1.1 Mining Sequence Data: Time-Series, Symbolic Sequences, and Biological Sequences

A **sequence** is an ordered list of events. Sequences may be categorized into three groups, based on the characteristics of the events they describe: (1) *time-series data*, (2) *symbolic sequence data*, and (3) *biological sequences*. Let's consider each type.

In **time-series data**, sequence data consist of long sequences of numeric data, recorded at equal time intervals (e.g., per minute, per hour, or per day). Time-series data can be generated by many natural and economic processes such as stock markets, and scientific, medical, or natural observations.

Symbolic sequence data consist of long sequences of event or nominal data, which typically are not observed at equal time intervals. For many such sequences, *gaps* (i.e., lapses between recorded events) do not matter much. Examples include customer shopping sequences and web click streams, as well as sequences of events in science and engineering and in natural and social developments.

Biological sequences include DNA and protein sequences. Such sequences are typically very long, and carry important, complicated, but hidden semantic meaning. Here, gaps are usually important.

Let's look into data mining for each of these sequence data types.

Similarity Search in Time-Series Data

A **time-series data set** consists of sequences of numeric values obtained over repeated measurements of time. The values are typically measured at equal time intervals (e.g., every minute, hour, or day). Time-series databases are popular in many applications such as stock market analysis, economic and sales forecasting, budgetary analysis, utility studies, inventory studies, yield projections, workload projections, and process and quality control. They are also useful for studying natural phenomena (e.g., atmosphere, temperature, wind, earthquake), scientific and engineering experiments, and medical treatments.

Unlike normal database queries, which find data that match a given query *exactly*, a **similarity search** finds data sequences that *differ only slightly* from the given query sequence. Many time-series similarity queries require **subsequence matching**, that is, finding a set of sequences that contain subsequences that are similar to a given query sequence.

For similarity search, it is often necessary to first perform *data or dimensionality reduction and transformation* of time-series data. Typical *dimensionality reduction* techniques include (1) the *discrete Fourier transform* (*DFT*), (2) *discrete wavelet transforms (DWT)*, and (3) *singular value decomposition* (*SVD*) based on *principle components analysis* (*PCA*). Because we touched on these concepts in Chapter 3, and because a thorough explanation is beyond the scope of this book, we will not go into great detail here. With such techniques, the data or signal is mapped to a signal in a *transformed space*. A small subset of the "strongest" transformed coefficients are saved as features.

These features form a *feature space*, which is a projection of the transformed space. Indices can be constructed on the original or transformed time-series data to speed up a search. For a query-based similarity search, techniques include normalization transformation, atomic matching (i.e., finding pairs of gap-free windows of a small length that are similar), window stitching (i.e., stitching similar windows to form pairs of large similar subsequences, allowing gaps between atomic matches), and subsequence ordering (i.e., linearly ordering the subsequence matches to determine whether enough similar pieces exist). Numerous software packages exist for a similarity search in time-series data.

Recently, researchers have proposed transforming time-series data into piecewise aggregate approximations so that the data can be viewed as a sequence of symbolic representations. The problem of similarity search is then transformed into one of matching subsequences in symbolic sequence data. We can identify *motifs* (i.e., frequently occurring sequential patterns) and build index or hashing mechanisms for an efficient search based on such motifs. Experiments show this approach is fast and simple, and has comparable search quality to that of DFT, DWT, and other dimensionality reduction methods.

Regression and Trend Analysis in Time-Series Data

Regression analysis of time-series data has been studied substantially in the fields of statistics and signal analysis. However, one may often need to go beyond pure regression

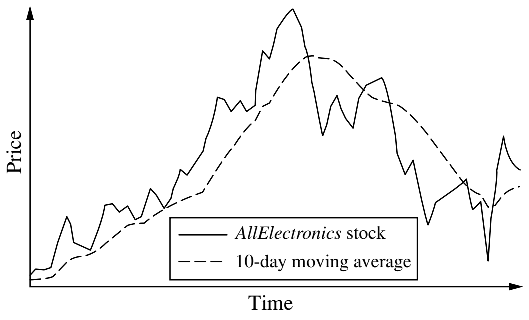


Figure 13.2 Time-series data for the stock price of *AllElectronics* over time. The *trend* is shown with a dashed curve, calculated by a moving average.

analysis and perform *trend analysis* for many practical applications. Trend analysis builds an integrated model using the following four major *components* or *movements* to characterize time-series data:

1. **Trend or long-term movements**: These indicate the general direction in which a time-series graph is moving over time, for example, using *weighted moving average* and the *least squares* methods to find *trend curves* such as the dashed curve indicated in Figure 13.2.
2. **Cyclic movements**: These are the long-term oscillations about a trend line or curve.
3. **Seasonal variations**: These are nearly identical patterns that a time series appears to follow during corresponding seasons of successive years such as holiday shopping seasons. For effective trend analysis, the data often need to be "deseasonalized" based on a **seasonal index** computed by autocorrelation.
4. **Random movements**: These characterize sporadic changes due to chance events such as labor disputes or announced personnel changes within companies.

Trend analysis can also be used for **time-series forecasting**, that is, finding a mathematical function that will approximately generate the historic patterns in a time series, and using it to make long-term or short-term predictions of future values. *ARIMA (auto-regressive integrated moving average)*, *long-memory time-series modeling*, and *autoregression* are popular methods for such analysis.

Sequential Pattern Mining in Symbolic Sequences

A **symbolic sequence** consists of an ordered set of elements or events, recorded with or without a concrete notion of time. There are many applications involving data of symbolic sequences such as customer shopping sequences, web click streams, program execution sequences, biological sequences, and sequences of events in science and engineering and in natural and social developments. Because biological sequences carry very complicated semantic meaning and pose many challenging research issues, most investigations are conducted in the field of bioinformatics.

Sequential pattern mining has focused extensively on mining symbolic sequences. A sequential pattern is a frequent subsequence existing in a single sequence or a set of sequences. A sequence $\alpha = \langle a_1 a_2 \cdots a_n \rangle$ is a **subsequence** of another sequence $\beta = \langle b_1 b_2 \cdots b_m \rangle$ if there exist integers $1 \leq j_1 < j_2 < \cdots < j_n \leq m$ such that $a_1 \subseteq b_{j_1}$, $a_2 \subseteq b_{j_2}, \ldots, a_n \subseteq b_{j_n}$. For example, if $\alpha = \langle \{ab\}, d \rangle$ and $\beta = \langle \{abc\}, \{be\}, \{de\}, a \rangle$, where a, b, c, d, and e are items, then α is a subsequence of β. Mining of sequential patterns consists of mining the set of subsequences that are frequent in one sequence or a set of sequences. Many scalable algorithms have been developed as a result of extensive studies in this area. Alternatively, we can mine only the *set of closed* sequential patterns, where a sequential pattern s is **closed** if there exists no sequential pattern s', where s is a *proper* subsequence of s', and s' has the same (frequency) support as s. Similar to its frequent pattern mining counterpart, there are also studies on efficient mining of **multidimensional, multilevel sequential patterns**.

As with constraint-based frequent pattern mining, user-specified constraints can be used to reduce the search space in sequential pattern mining and derive only the patterns that are of interest to the user. This is referred to as **constraint-based sequential pattern mining**. Moreover, we may relax constraints or enforce additional constraints on the problem of sequential pattern mining to derive different kinds of patterns from sequence data. For example, we can enforce gap constraints so that the patterns derived contain only consecutive subsequences or subsequences with very small gaps. Alternatively, we may derive periodic sequential patterns by folding events into proper-size windows and finding recurring subsequences in these windows. Another approach derives *partial order patterns* by relaxing the requirement of strict sequential ordering in the mining of subsequence patterns. Besides mining partial order patterns, sequential pattern mining methodology can also be extended to mining trees, lattices, episodes, and some other ordered patterns.

Sequence Classification

Most classification methods perform model construction based on feature vectors. However, sequences do not have explicit features. Even with sophisticated feature selection techniques, the dimensionality of potential features can still be very high and the sequential nature of features is difficult to capture. This makes sequence classification a challenging task.

Sequence classification methods can be organized into three categories: (1) feature-based classification, which transforms a sequence into a feature vector and then applies conventional classification methods; (2) sequence distance–based classification, where the distance function that measures the similarity between sequences determines the quality of the classification significantly; and (3) model-based classification such as using hidden Markov model (HMM) or other statistical models to classify sequences.

For time-series or other numeric-valued data, the feature selection techniques for symbolic sequences cannot be easily applied to time-series data without discretization. However, discretization can cause information loss. A recently proposed time-series *shapelets method* uses the time-series subsequences that can maximally represent a class as the features. It achieves quality classification results.

Alignment of Biological Sequences

Biological sequences generally refer to sequences of nucleotides or amino acids. **Biological sequence analysis** compares, aligns, indexes, and analyzes biological sequences and thus plays a crucial role in bioinformatics and modern biology.

Sequence alignment is based on the fact that all living organisms are related by evolution. This implies that the nucleotide (DNA, RNA) and protein sequences of species that are closer to each other in evolution should exhibit more similarities. An **alignment** is the process of lining up sequences to achieve a maximal identity level, which also expresses the degree of similarity between sequences. Two sequences are **homologous** if they share a common ancestor. The degree of similarity obtained by sequence alignment can be useful in determining the possibility of homology between two sequences. Such an alignment also helps determine the relative positions of multiple species in an evolution tree, which is called a **phylogenetic tree**.

The problem of alignment of biological sequences can be described as follows: *Given two or more input biological sequences, identify similar sequences with long conserved subsequences.* If the number of sequences to be aligned is exactly two, the problem is known as **pairwise sequence alignment**; otherwise, it is **multiple sequence alignment**. The sequences to be compared and aligned can be either nucleotides (DNA/RNA) or amino acids (proteins). For nucleotides, two symbols align if they are identical. However, for amino acids, two symbols align if they are identical, or if one can be derived from the other by substitutions that are likely to occur in nature. There are two kinds of alignments: *local alignments* and *global alignments*. The former means that only portions of the sequences are aligned, whereas the latter requires alignment over the entire length of the sequences.

For either nucleotides or amino acids, insertions, deletions, and substitutions occur in nature with different probabilities. **Substitution matrices** are used to represent the probabilities of substitutions of nucleotides or amino acids and probabilities of insertions and deletions. Usually, we use the gap character, −, to indicate positions where it is preferable not to align two symbols. To evaluate the quality of alignments, a *scoring* mechanism is typically defined, which usually counts identical or similar symbols as positive scores and gaps as negative ones. The algebraic sum of the scores is taken as the alignment measure. The goal of alignment is to achieve the maximal score among all the possible alignments. However, it is very expensive (more exactly, an NP-hard problem) to find optimal alignment. Therefore, various heuristic methods have been developed to find suboptimal alignments.

The dynamic programming approach is commonly used for sequence alignments. Among many available analysis packages, BLAST (Basic Local Alignment Search Tool) is one of the most popular tools in biosequence analysis.

Hidden Markov Model for Biological Sequence Analysis

Given a biological sequence, biologists would like to analyze what that sequence represents. To represent the structure or statistical regularities of sequence classes, biologists construct various probabilistic models such as *Markov chains* and *hidden Markov models*. In both models, the probability of a state depends only on that of the previous state; therefore, they are particularly useful for the analysis of biological sequence data. The most common methods for constructing hidden Markov models are the forward algorithm, the Viterbi algorithm, and the Baum-Welch algorithm. Given a sequence of symbols, x, the *forward algorithm* finds the probability of obtaining x in the model; the *Viterbi algorithm* finds the most probable path (corresponding to x) through the model, whereas the *Baum-Welch algorithm* learns or adjusts the model parameters so as to best explain a set of training sequences.

13.1.2 Mining Graphs and Networks

Graphs represents a more general class of structures than sets, sequences, lattices, and trees. There is a broad range of graph applications on the Web and in social networks, information networks, biological networks, bioinformatics, chemical informatics, computer vision, and multimedia and text retrieval. Hence, graph and network mining have become increasingly important and heavily researched. We overview the following major themes: (1) graph pattern mining; (2) statistical modeling of networks; (3) data cleaning, integration, and validation by network analysis; (4) clustering and classification of graphs and homogeneous networks; (5) clustering, ranking, and classification of heterogeneous networks; (6) role discovery and link prediction in information networks; (7) similarity search and OLAP in information networks; and (8) evolution of information networks.

Graph Pattern Mining

Graph pattern mining is the mining of *frequent subgraphs* (also called **(sub)graph patterns**) in one or a set of graphs. Methods for mining graph patterns can be categorized into Apriori-based and pattern growth–based approaches. Alternatively, we can mine the set of *closed graphs* where a graph g is *closed* if there exists no proper supergraph g' that carries the same support count as g. Moreover, there are many *variant graph patterns*, including approximate frequent graphs, coherent graphs, and dense graphs. User-specified constraints can be pushed deep into the graph pattern mining process to improve mining efficiency.

Graph pattern mining has many interesting applications. For example, it can be used to generate compact and effective *graph index structures* based on the concept of frequent and discriminative graph patterns. Approximate *structure similarity search* can be achieved by exploring graph index structures and multiple graph features. Moreover, classification of graphs can also be performed effectively using frequent and discriminative subgraphs as features.

Statistical Modeling of Networks

A **network** consists of a set of *nodes*, each corresponding to an *object* associated with a set of properties, and a set of *edges* (or *links*) connecting those nodes, representing relationships between objects. A network is **homogeneous** if all the nodes and links are of the same type, such as a friend network, a coauthor network, or a web page network. A network is **heterogeneous** if the nodes and links are of different types, such as publication networks (linking together authors, conferences, papers, and contents), and health-care networks (linking together doctors, nurses, patients, diseases, and treatments).

Researchers have proposed multiple statistical models for modeling homogeneous networks. The most well-known generative models are the random graph model (i.e., the Erdös-Rényi model), the Watts-Strogatz model, and the scale-free model. The scale-free model assumes that the network follows the *power law distribution* (also known as the *Pareto distribution* or the *heavy-tailed distribution*). In most large-scale social networks, a **small-world phenomenon** is observed, that is, the network can be characterized as having a high degree of local clustering for a small fraction of the nodes (i.e., these nodes are interconnected with one another), while being no more than a few degrees of separation from the remaining nodes.

Social networks exhibit certain evolutionary characteristics. They tend to follow the **densification power law**, which states that networks become increasingly *dense* over time. **Shrinking diameter** is another characteristic, where the effective diameter often *decreases* as the network grows. Node *out-degrees* and *in-degrees* typically follow a heavy-tailed distribution.

Data Cleaning, Integration, and Validation by Information Network Analysis

Real-world data are often incomplete, noisy, uncertain, and unreliable. Information redundancy may exist among the multiple pieces of data that are interconnected in a large network. Information redundancy can be explored in such networks to perform quality data cleaning, data integration, information validation, and trustability analysis by network analysis. For example, we can distinguish authors who share the same names by examining the networked connections with other heterogeneous objects such as coauthors, publication venues, and terms. In addition, we can identify inaccurate author information presented by booksellers by exploring a network built based on author information provided by multiple booksellers.

Sophisticated information network analysis methods have been developed in this direction, and in many cases, portions of the data serve as the "training set." That is, relatively clean and reliable data or a consensus of data from multiple information providers can be used to help consolidate the remaining, unreliable portions of the data. This reduces the costly efforts of labeling the data by hand and of training on massive, dynamic, real-world data sets.

Clustering and Classification of Graphs and Homogeneous Networks

Large graphs and networks have cohesive structures, which are often hidden among their massive, interconnected nodes and links. Cluster analysis methods have been developed on large networks to uncover network structures, discover hidden communities, hubs, and outliers based on network topological structures and their associated properties. Various kinds of network clustering methods have been developed and can be categorized as either partitioning, hierarchical, or density-based algorithms. Moreover, given human-labeled training data, the discovery of network structures can be guided by human-specified heuristic constraints. Supervised classification and semi-supervised classification of networks are recent hot topics in the data mining research community.

Clustering, Ranking, and Classification of Heterogeneous Networks

A heterogeneous network contains interconnected nodes and links of different types. Such interconnected structures contain rich information, which can be used to mutually enhance nodes and links, and propagate knowledge from one type to another. Clustering and ranking of such heterogeneous networks can be performed hand-in-hand in the context that highly ranked nodes/links in a cluster may contribute more than their lower-ranked counterparts in the evaluation of the cohesiveness of a cluster. Clustering may help consolidate the high ranking of objects/links dedicated to the cluster. Such mutual enhancement of ranking and clustering prompted the development of an algorithm called RankClus. Moreover, users may specify different ranking rules or present labeled nodes/links for certain data types. Knowledge of one type can be propagated to other types. Such propagation reaches the nodes/links of the same type via heterogeneous-type connections. Algorithms have been developed for supervised learning and semi-supervised learning in heterogeneous networks.

Role Discovery and Link Prediction in Information Networks

There exist many hidden roles or relationships among different nodes/links in a heterogeneous network. Examples include advisor–advisee and leader–follower relationships in a research publication network. To discover such hidden roles or relationships, experts can specify constraints based on their background knowledge. Enforcing such constraints may help cross-checking and validation in large interconnected networks. Information redundancy in a network can often be used to help weed out objects/links that do not follow such constraints.

Similarly, *link prediction* can be performed based on the assessment of the ranking of the expected relationships among the candidate nodes/links. For example, we may predict which papers an author may write, read, or cite, based on the author's recent publication history and the trend of research on similar topics. Such studies often require analyzing the proximity of network nodes/links and the trends and connections of their similar neighbors. Roughly speaking, people refer to link prediction as **link mining**; however, link mining covers additional tasks including *link-based object classification*, *object type prediction*, *link type prediction, link existence prediction*, *link cardinality estimation*, and *object reconciliation* (which predicts whether two objects are, in fact, the same). It also includes *group detection* (which clusters objects), as well as *subgraph identification* (which finds characteristic subgraphs within networks) and *metadata mining* (which uncovers schema-type information regarding unstructured data).

Similarity Search and OLAP in Information Networks

Similarity search is a primitive operation in database and web search engines. A heterogeneous information network consists of multityped, interconnected objects. Examples include bibliographic networks and social media networks, where two objects are considered similar if they are linked in a similar way with multityped objects. In general, object similarity within a network can be determined based on network structures and object properties, and with similarity measures. Moreover, network clusters and hierarchical network structures help organize objects in a network and identify subcommunities, as well as facilitate similarity search. Furthermore, similarity can be defined differently per user. By considering different linkage paths, we can derive various similarity semantics in a network, which is known as *path-based similarity*.

By organizing networks based on the notion of similarity and clusters, we can generate multiple hierarchies within a network. Online analytical processing (OLAP) can then be performed. For example, we can drill down or dice information networks based on different levels of abstraction and different angles of views. OLAP operations may generate multiple, interrelated networks. The relationships among such networks may disclose interesting hidden semantics.

Evolution of Social and Information Networks

Networks are dynamic and constantly evolving. Detecting evolving communities and evolving regularities or anomalies in homogeneous or heterogeneous networks can help people better understand the structural evolution of networks and predict trends and irregularities in evolving networks. For homogeneous networks, the evolving communities discovered are subnetworks consisting of objects of the same type such as a set of friends or coauthors. However, for heterogeneous networks, the communities discovered are subnetworks consisting of objects of different types, such as a connected set of papers, authors, venues, and terms, from which we can also derive a set of evolving objects for each type, like evolving authors and themes.

13.1.3 Mining Other Kinds of Data

In addition to sequences and graphs, there are many other kinds of semi-structured or unstructured data, such as spatiotemporal, multimedia, and hypertext data, which have interesting applications. Such data carry various kinds of semantics, are either stored in or dynamically streamed through a system, and call for specialized data mining methodologies. Thus, mining multiple kinds of data, including *spatial data, spatiotemporal data, cyber-physical system data, multimedia data, text data*, *web data*, and *data streams*, are increasingly important tasks in data mining. In this subsection, we overview the methodologies for mining these kinds of data.

Mining Spatial Data

Spatial data mining discovers patterns and knowledge from spatial data. Spatial data, in many cases, refer to geospace-related data stored in geospatial data repositories. The data can be in "vector" or "raster" formats, or in the form of imagery and geo-referenced multimedia. Recently, large *geographic data warehouses* have been constructed by integrating thematic and geographically referenced data from multiple sources. From these, we can construct *spatial data cubes* that contain spatial dimensions and measures, and support *spatial OLAP* for *multidimensional spatial data analysis.* Spatial data mining can be performed on spatial data warehouses, spatial databases, and other geospatial data repositories. Popular topics on geographic knowledge discovery and spatial data mining include *mining spatial associations and co-location patterns*, *spatial clustering*, *spatial classification*, *spatial modeling*, and *spatial trend and outlier analysis.*

Mining Spatiotemporal Data and Moving Objects

Spatiotemporal data are data that relate to both space and time. **Spatiotemporal data mining** refers to the process of discovering patterns and knowledge from spatiotemporal data. Typical examples of spatiotemporal data mining include discovering the evolutionary history of cities and lands, uncovering weather patterns, predicting earthquakes and hurricanes, and determining global warming trends. Spatiotemporal data mining has become increasingly important and has far-reaching implications, given the popularity of mobile phones, GPS devices, Internet-based map services, weather services, and digital Earth, as well as satellite, RFID, sensor, wireless, and video technologies.

Among many kinds of spatiotemporal data, *moving-object data* (i.e., data about moving objects) are especially important. For example, animal scientists attach telemetry equipment on wildlife to analyze ecological behavior, mobility managers embed GPS in cars to better monitor and guide vehicles, and meteorologists use weather satellites and radars to observe hurricanes. Massive-scale moving-object data are becoming rich, complex, and ubiquitous. Examples of **moving-object data mining** include mining *movement patterns of multiple moving objects* (i.e., the discovery of relationships among multiple moving objects such as moving clusters, leaders and followers, merge, convoy, swarm, and pincer, as well as other collective movement patterns). Other examples of moving-object data mining include mining *periodic patterns* for one or a set of moving objects, and mining *trajectory patterns*, *clusters*, *models*, and *outliers*.

Mining Cyber-Physical System Data

A **cyber-physical system** (CPS) typically consists of a large number of interacting physical and information components. CPS systems may be interconnected so as to form large heterogeneous *cyber-physical networks*. Examples of cyber-physical networks include a patient care system that links a patient monitoring system with a network of patient/medical information and an emergency handling system; a transportation system that links a transportation monitoring network, consisting of many sensors and video cameras, with a traffic information and control system; and a battlefield commander system that links a sensor/reconnaissance network with a battlefield information analysis system. Clearly, cyber-physical systems and networks will be ubiquitous and form a critical component of modern information infrastructure.

Data generated in cyber-physical systems are dynamic, volatile, noisy, inconsistent, and interdependent, containing rich spatiotemporal information, and they are critically important for real-time decision making. In comparison with typical spatiotemporal data mining, mining cyber-physical data requires linking the current situation with a large information base, performing real-time calculations, and returning prompt responses. Research in the area includes rare-event detection and anomaly analysis in cyber-physical data streams, reliability and trustworthiness in cyber-physical data analysis, effective spatiotemporal data analysis in cyber-physical networks, and the integration of stream data mining with real-time automated control processes.

Mining Multimedia Data

Multimedia data mining is the discovery of interesting patterns from multimedia databases that store and manage large collections of multimedia objects, including image data, video data, audio data, as well as sequence data and hypertext data containing text, text markups, and linkages. Multimedia data mining is an interdisciplinary field that integrates image processing and understanding, computer vision, data mining, and pattern recognition. Issues in multimedia data mining include *content-based retrieval and similarity search*, and *generalization and multidimensional analysis*. Multimedia data cubes contain additional dimensions and measures for multimedia information. Other topics in multimedia mining include *classification and prediction analysis*, *mining associations*, and *video and audio data mining* (Section 13.2.3).

Mining Text Data

Text mining is an interdisciplinary field that draws on information retrieval, data mining, machine learning, statistics, and computational linguistics. A substantial portion of information is stored as text such as news articles, technical papers, books, digital libraries, email messages, blogs, and web pages. Hence, research in text mining has been very active. An important goal is to derive high-quality information from text. This is typically done through the discovery of patterns and trends by means such as statistical pattern learning, topic modeling, and statistical language modeling. Text mining usually requires structuring the input text (e.g., parsing, along with the addition of some derived linguistic features and the removal of others, and subsequent insertion into a database). This is followed by deriving patterns within the structured data, and evaluation and interpretation of the output. "High quality" in text mining usually refers to a combination of relevance, novelty, and interestingness.

Typical text mining tasks include text categorization, text clustering, concept/entity extraction, production of granular taxonomies, sentiment analysis, document summarization, and entity-relation modeling (i.e., learning relations between named entities). Other examples include multilingual data mining, multidimensional text analysis, contextual text mining, and trust and evolution analysis in text data, as well as text mining applications in security, biomedical literature analysis, online media analysis, and analytical customer relationship management. Various kinds of text mining and analysis software and tools are available in academic institutions, open-source forums, and industry. Text mining often also uses WordNet, Sematic Web, Wikipedia, and other information sources to enhance the understanding and mining of text data.

Mining Web Data

The World Wide Web serves as a huge, widely distributed, global information center for news, advertisements, consumer information, financial management, education, government, and e-commerce. It contains a rich and dynamic collection of information about web page contents with hypertext structures and multimedia, hyperlink information, and access and usage information, providing fertile sources for data mining. **Web mining** is the application of data mining techniques to discover patterns, structures, and knowledge from the Web. According to analysis targets, web mining can be organized into three main areas: *web content mining*, *web structure mining*, and *web usage mining*.

Web content mining analyzes web content such as text, multimedia data, and structured data (within web pages or linked across web pages). This is done to understand the content of web pages, provide scalable and informative keyword-based page indexing, entity/concept resolution, web page relevance and ranking, web page content summaries, and other valuable information related to web search and analysis. Web pages can reside either on the *surface web* or on the *deep Web*. The *surface web* is that portion of the Web that is indexed by typical search engines. The *deep Web* (or *hidden Web*) refers to web content that is not part of the surface web. Its contents are provided by underlying database engines.

Web content mining has been studied extensively by researchers, search engines, and other web service companies. Web content mining can build links across multiple web pages for individuals; therefore, it has the potential to inappropriately disclose personal information. Studies on privacy-preserving data mining address this concern through the development of techniques to protect personal privacy on the Web.

Web structure mining is the process of using graph and network mining theory and methods to analyze the nodes and connection structures on the Web. It extracts patterns from hyperlinks, where a hyperlink is a structural component that connects a web page to another location. It can also mine the document structure within a page (e.g., analyze the treelike structure of page structures to describe HTML or XML tag usage). Both kinds of web structure mining help us understand web contents and may also help transform web contents into relatively structured data sets.

Web usage mining is the process of extracting useful information (e.g., user click streams) from server logs. It finds patterns related to general or particular groups of users; understands users' search patterns, trends, and associations; and predicts what users are looking for on the Internet. It helps improve search efficiency and effectiveness, as well as promotes products or related information to different groups of users at the right time. Web search companies routinely conduct web usage mining to improve their quality of service.

Mining Data Streams

Stream data refer to data that flow into a system in vast volumes, change dynamically, are possibly infinite, and contain multidimensional features. Such data cannot be stored in traditional database systems. Moreover, most systems may only be able to read the stream once in sequential order. This poses great challenges for the effective mining of stream data. Substantial research has led to progress in the development of efficient methods for mining data streams, in the areas of mining frequent and sequential patterns, multidimensional analysis (e.g., the construction of stream cubes), classification, clustering, outlier analysis, and the online detection of rare events in data streams. The general philosophy is to develop single-scan or a-few-scan algorithms using limited computing and storage capabilities.

This includes collecting information about stream data in sliding windows or *tilted time windows* (where the most recent data are registered at the finest granularity and the more distant data are registered at a coarser granularity), and exploring techniques like microclustering, limited aggregation, and approximation. Many applications of stream data mining can be explored—for example, real-time detection of anomalies in computer network traffic, botnets, text streams, video streams, power-grid flows, web searches, sensor networks, and cyber-physical systems.

13.2 Other Methodologies of Data Mining

Due to the broad scope of data mining and the large variety of data mining methodologies, not all methodologies of data mining can be thoroughly covered in this book. In this section, we briefly discuss several interesting methodologies that were not fully addressed in the previous chapters. These methodologies are listed in Figure 13.3.

13.2.1 Statistical Data Mining

The data mining techniques described in this book are primarily drawn from computer science disciplines, including data mining, machine learning, data warehousing, and algorithms. They are designed for the efficient handling of huge amounts of data that are

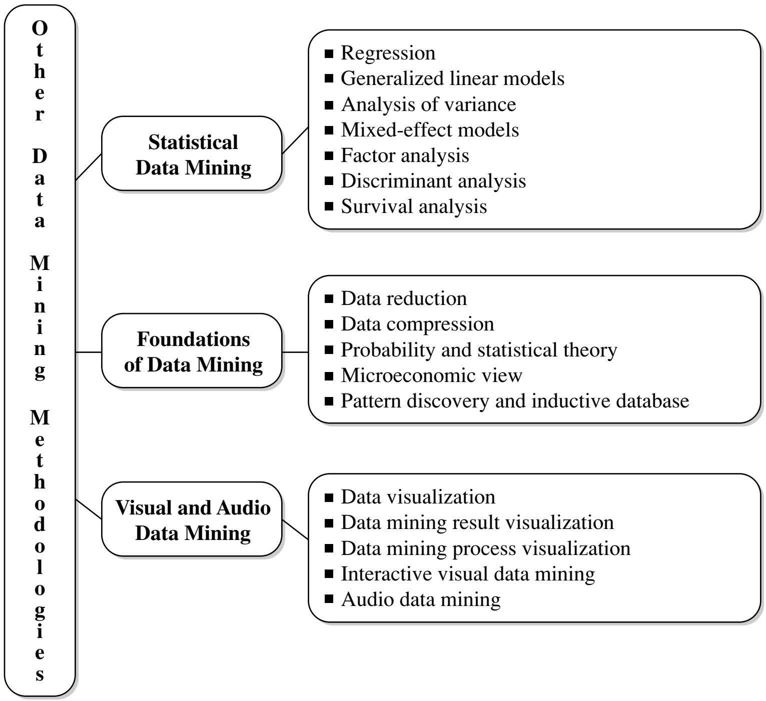

Other Data Mining Methodologies
Statistical Data Mining
Regression
Generalized linear models
Analysis of variance
Mixed-effect models
Factor analysis
Discriminant analysis
Survival analysis
Foundations of Data Mining
Data reduction
Data compression
Probability and statistical theory
Microeconomic view
Pattern discovery and inductive database
Visual and Audio Data Mining
Data visualization
Data mining result visualization
Data mining process visualization
Interactive visual data mining
Audio data mining

Figure 13.3 Other data mining methodologies.

typically multidimensional and possibly of various complex types. There are, however, many well-established statistical techniques for data analysis, particularly for numeric data. These techniques have been applied extensively to scientific data (e.g., data from experiments in physics, engineering, manufacturing, psychology, and medicine), as well as to data from economics and the social sciences. Some of these techniques, such as principal components analysis (Chapter 3) and clustering (Chapters 10 and 11), have already been addressed in this book. A thorough discussion of major statistical methods for data analysis is beyond the scope of this book; however, several methods are mentioned here for the sake of completeness. Pointers to these techniques are provided in the bibliographic notes (Section 13.8).

- **Regression**: In general, these methods are used to predict the value of a *response* (dependent) variable from one or more *predictor* (independent) variables, where the variables are numeric. There are various forms of regression, such as linear, multiple, weighted, polynomial, nonparametric, and robust (robust methods are useful when errors fail to satisfy normalcy conditions or when the data contain significant outliers).
- **Generalized linear models**: These models, and their generalization (*generalized additive models*), allow a *categorical* (nominal) response variable (or some transformation

of it) to be related to a set of predictor variables in a manner similar to the modeling of a numeric response variable using linear regression. Generalized linear models include logistic regression and Poisson regression.

- **Analysis of variance**: These techniques analyze experimental data for two or more populations described by a numeric response variable and one or more categorical variables (*factors*). In general, an ANOVA (single-factor analysis of variance) problem involves a comparison of *k* population or treatment means to determine if at least two of the means are different. More complex ANOVA problems also exist.
- **Mixed-effect models**: These models are for analyzing grouped data—data that can be classified according to one or more grouping variables. They typically describe relationships between a response variable and some covariates in data grouped according to one or more factors. Common areas of application include multilevel data, repeated measures data, block designs, and longitudinal data.
- **Factor analysis**: This method is used to determine which variables are combined to generate a given factor. For example, for many psychiatric data, it is not possible to measure a certain factor of interest directly (e.g., intelligence); however, it is often possible to measure other quantities (e.g., student test scores) that reflect the factor of interest. Here, none of the variables is designated as dependent.
- **Discriminant analysis**: This technique is used to predict a categorical response variable. Unlike generalized linear models, it assumes that the independent variables follow a multivariate normal distribution. The procedure attempts to determine several discriminant functions (linear combinations of the independent variables) that discriminate among the groups defined by the response variable. Discriminant analysis is commonly used in social sciences.
- **Survival analysis**: Several well-established statistical techniques exist for survival analysis. These techniques originally were designed to predict the probability that a patient undergoing a medical treatment would survive at least to time t. Methods for survival analysis, however, are also commonly applied to manufacturing settings to estimate the life span of industrial equipment. Popular methods include Kaplan-Meier estimates of survival, Cox proportional hazards regression models, and their extensions.
- **Quality control**: Various statistics can be used to prepare charts for quality control, such as Shewhart charts and CUSUM charts (both of which display group summary statistics). These statistics include the mean, standard deviation, range, count, moving average, moving standard deviation, and moving range.

13.2.2 Views on Data Mining Foundations

Research on the theoretical foundations of data mining has yet to mature. A solid and systematic theoretical foundation is important because it can help provide a coherent framework for the development, evaluation, and practice of data mining technology. Several theories for the basis of data mining include the following:

- **Data reduction**: In this theory, the basis of data mining is to reduce the data representation. Data reduction trades accuracy for speed in response to the need to obtain quick approximate answers to queries on very large databases. Data reduction techniques include singular value decomposition (the driving element behind principal components analysis), wavelets, regression, log-linear models, histograms, clustering, sampling, and the construction of index trees.
- **Data compression**: According to this theory, the basis of data mining is to compress the given data by encoding in terms of bits, association rules, decision trees, clusters, and so on. Encoding based on the *minimum description length principle* states that the "best" theory to infer from a data set is the one that minimizes the length of the theory and of the data when encoded, using the theory as a predictor for the data. This encoding is typically in bits.
- **Probability and statistical theory**: According to this theory, the basis of data mining is to discover joint probability distributions of random variables, for example, Bayesian belief networks or hierarchical Bayesian models.
- **Microeconomic view**: The microeconomic view considers data mining as the task of finding patterns that are interesting only to the extent that they can be used in the decision-making process of some enterprise (e.g., regarding marketing strategies and production plans). This view is one of utility, in which patterns are considered interesting if they can be acted on. Enterprises are regarded as facing optimization problems, where the object is to maximize the utility or value of a decision. In this theory, data mining becomes a nonlinear optimization problem.
- **Pattern discovery and inductive databases**: In this theory, the basis of data mining is to discover patterns occurring in the data such as associations, classification models, sequential patterns, and so on. Areas such as machine learning, neural network, association mining, sequential pattern mining, clustering, and several other subfields contribute to this theory. A knowledge base can be viewed as a database consisting of data and patterns. A user interacts with the system by querying the data and the theory (i.e., patterns) in the knowledge base. Here, the knowledge base is actually an inductive database.

These theories are not mutually exclusive. For example, pattern discovery can also be seen as a form of data reduction or data compression. Ideally, a theoretical framework should be able to model typical data mining tasks (e.g., association, classification, and clustering), have a probabilistic nature, be able to handle different forms of data, and consider the iterative and interactive essence of data mining. Further efforts are required to establish a well-defined framework for data mining that satisfies these requirements.

13.2.3 Visual and Audio Data Mining

Visual data mining discovers implicit and useful knowledge from large data sets using data and/or knowledge visualization techniques. The human visual system is controlled by the eyes and brain, the latter of which can be thought of as a powerful, highly parallel processing and reasoning engine containing a large knowledge base. Visual data mining essentially combines the power of these components, making it a highly attractive and effective tool for the comprehension of data distributions, patterns, clusters, and outliers in data.

Visual data mining can be viewed as an integration of two disciplines: data visualization and data mining. It is also closely related to computer graphics, multimedia systems, human–computer interaction, pattern recognition, and high-performance computing. In general, data visualization and data mining can be integrated in the following ways:

- **Data visualization**: Data in a database or data warehouse can be viewed at different granularity or abstraction levels, or as different combinations of attributes or dimensions. Data can be presented in various visual forms, such as boxplots, 3-D cubes, data distribution charts, curves, surfaces, and link graphs, as shown in the data visualization section of Chapter 2. Figures 13.4 and 13.5 from StatSoft show

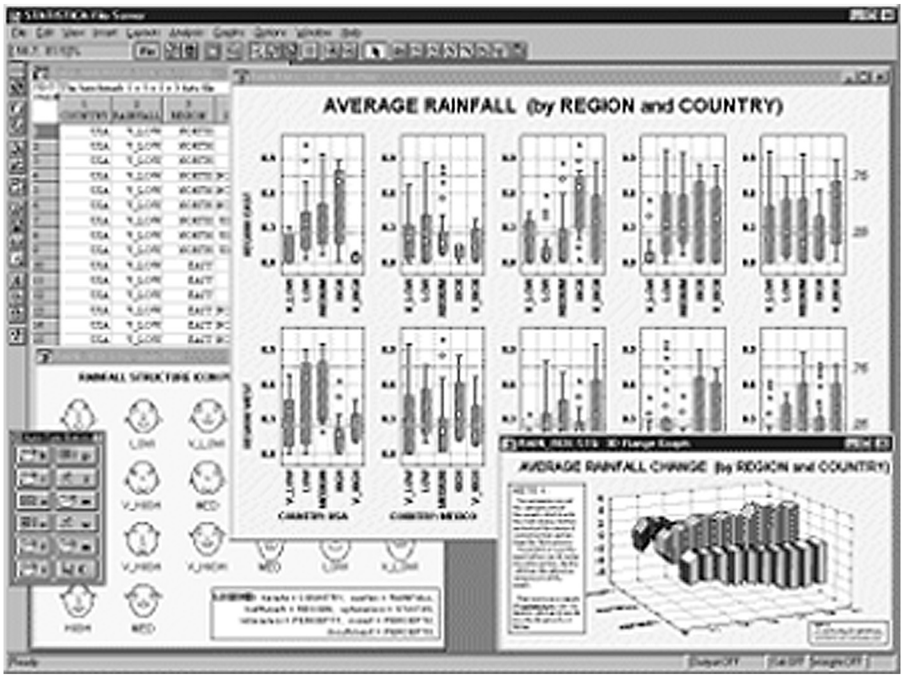

AVERAGE RAINFALL (by REGION and COUNTRY)
RAINFALL STRUCTURE ICONS
AVERAGE RAINFALL CHANGE (by REGION and COUNTRY)
COUNTRY: USA
COUNTRY: MEXICO

Figure 13.4 Boxplots showing multiple variable combinations in StatSoft. *Source: www.statsoft.com.*

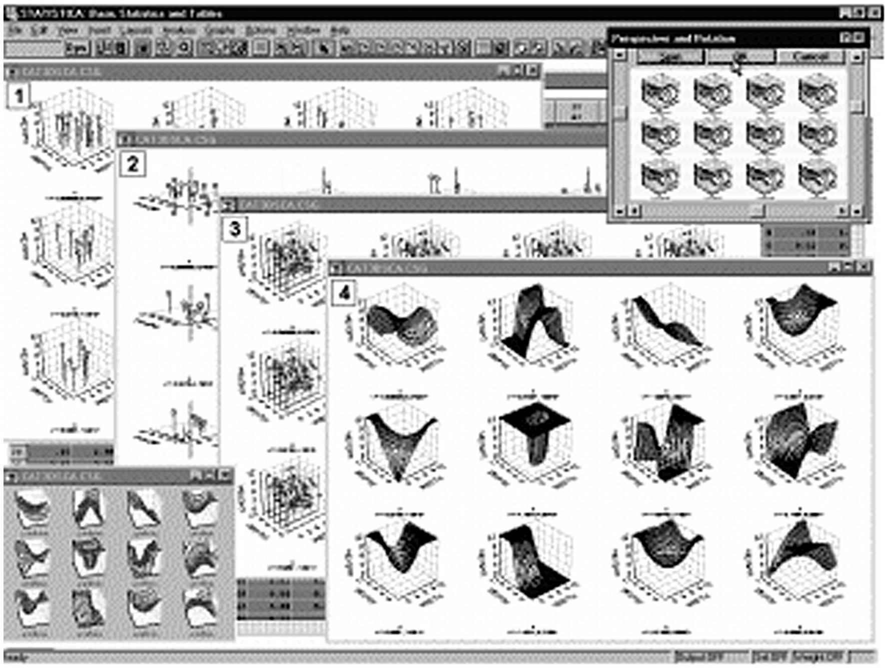
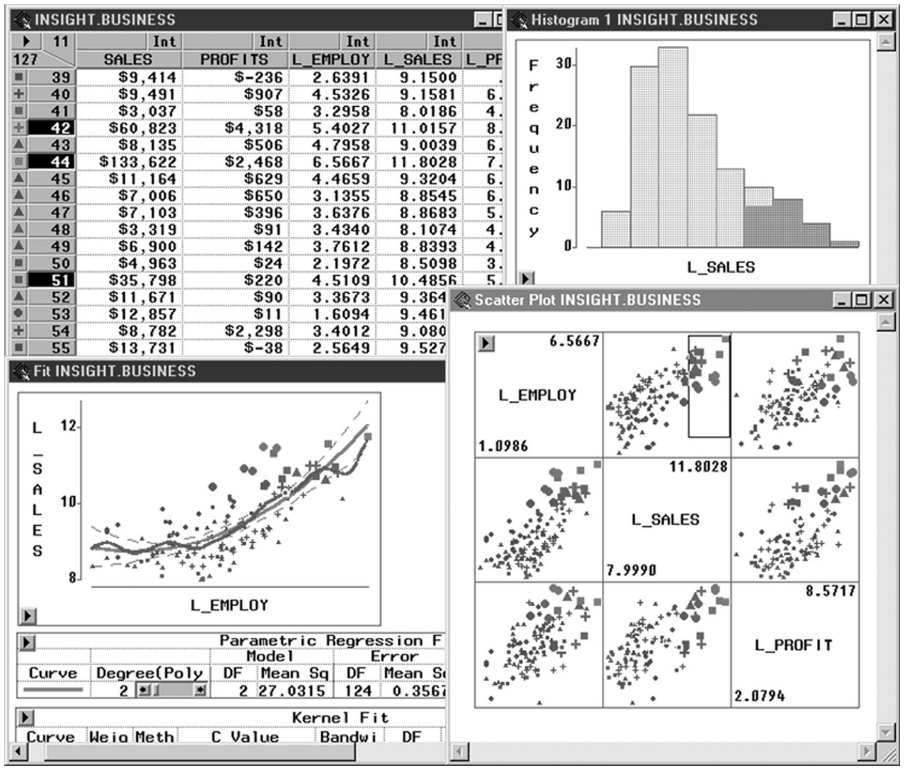


Figure 13.5 Multidimensional data distribution analysis in StatSoft. *Source: www.statsoft.com.*

data distributions in multidimensional space. Visual display can help give users a clear impression and overview of the data characteristics in a large data set.

- **Data mining result visualization**: Visualization of data mining results is the presentation of the results or knowledge obtained from data mining in visual forms. Such forms may include scatter plots and boxplots (Chapter 2), as well as decision trees, association rules, clusters, outliers, and generalized rules. For example, scatter plots are shown in Figure 13.6 from SAS Enterprise Miner. Figure 13.7, from MineSet, uses a plane associated with a set of pillars to describe a set of association rules mined from a database. Figure 13.8, also from MineSet, presents a decision tree. Figure 13.9, from IBM Intelligent Miner, presents a set of clusters and the properties associated with them.
- **Data mining process visualization**: This type of visualization presents the various processes of data mining in visual forms so that users can see how the data are extracted and from which database or data warehouse they are extracted, as well as how the selected data are cleaned, integrated, preprocessed, and mined. Moreover, it may also show which method is selected for data mining, where the results are stored, and how they may be viewed. Figure 13.10 shows a visual presentation of data mining processes by the Clementine data mining system.



11	Int	Int	Int	Int	
127	SALES	PROFITS	L_EMPLOY	L_SALES	L_PF
39	$9,414	$-236	2.6391	9.1500	.
40	$9,491	$907	4.5326	9.1581	6.
41	$3,037	$58	3.2958	8.0186	4.
42	$60,823	$4,318	5.4027	11.0157	8.
43	$8,135	$506	4.7958	9.0039	6.
44	$133,622	$2,468	6.5667	11.8028	7.
45	$11,164	$629	4.4659	9.3204	6.
46	$7,006	$650	3.1355	8.8545	6.
47	$7,103	$396	3.6376	8.8683	5.
48	$3,319	$91	3.4340	8.1074	4.
49	$6,900	$142	3.7612	8.8393	4.
50	$4,963	$24	2.1972	8.5098	3.
51	$35,798	$220	4.5109	10.4856	5.
52	$11,671	$90	3.3673	9.364	
53	$12,857	$11	1.6094	9.461	
54	$8,782	$2,298	3.4012	9.080	
55	$13,731	$-38	2.5649	9.527	

Parametric Regression F

		Model		Error	
Curve	Degree(Poly	DF	Mean Sq	DF	Mean S
	2	2	27.0315	124	0.3567

Kernel Fit

Curve	Weig	Meth	C Value	Bandwi	DF

Figure 13.6 Visualization of data mining results in SAS Enterprise Miner.

- **Interactive visual data mining**: In (interactive) visual data mining, visualization tools can be used in the data mining process to help users make smart data mining decisions. For example, the data distribution in a set of attributes can be displayed using colored sectors (where the whole space is represented by a circle). This display helps users determine which sector should first be selected for classification and where a good split point for this sector may be. An example of this is shown in Figure 13.11, which is the output of a perception-based classification (PBC) system developed at the University of Munich.

Audio data mining uses audio signals to indicate the patterns of data or the features of data mining results. Although visual data mining may disclose interesting patterns using graphical displays, it requires users to concentrate on watching patterns and identifying interesting or novel features within them. This can sometimes be quite tiresome. If patterns can be transformed into sound and music, then instead of watching pictures, we can listen to pitchs, rhythm, tune, and melody to identify anything interesting or unusual. This may relieve some of the burden of visual concentration and be more

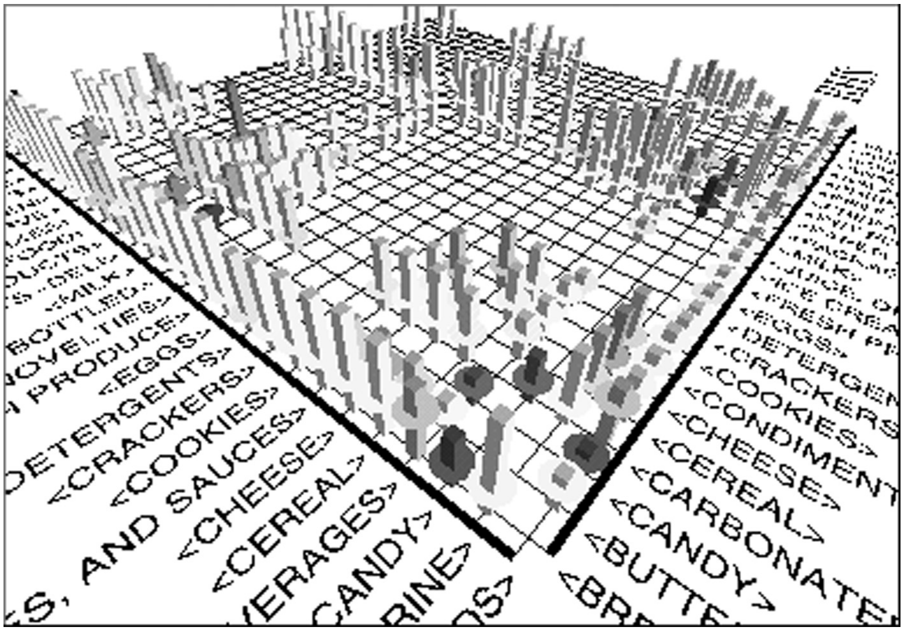


Figure 13.7 Visualization of association rules in MineSet.

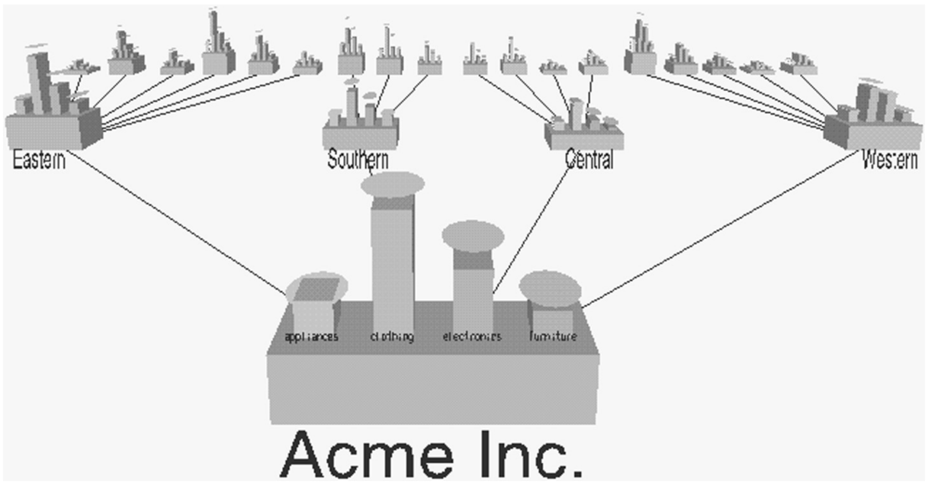


Figure 13.8 Visualization of a decision tree in MineSet.

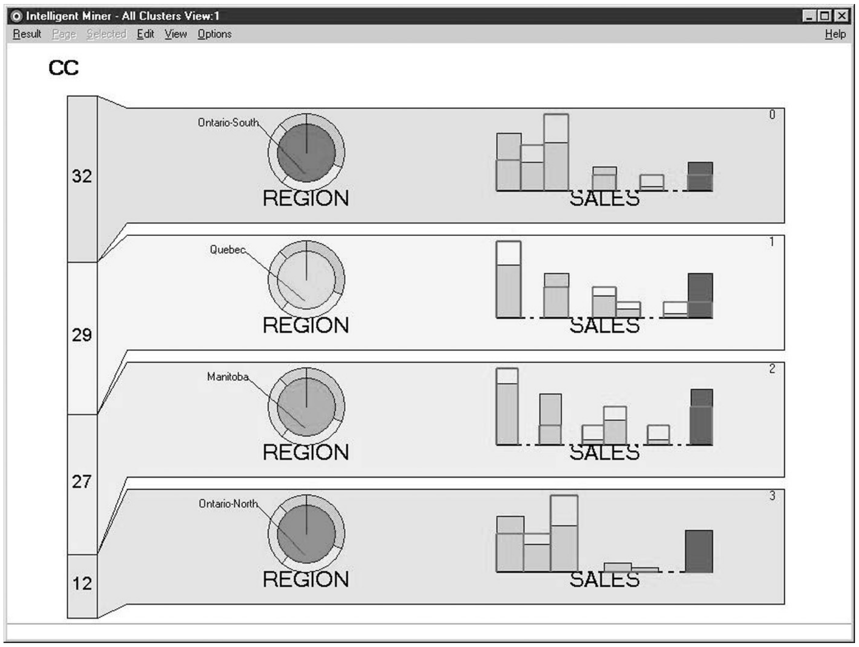

Intelligent Miner - All Clusters View:1
Result Page Selected Edit View Options Help
CC
32
29
27
12
Ontario-South
Quebec
Manitoba
Ontario-North
REGION
SALES
0
1
2
3

Figure 13.9 Visualization of cluster groupings in IBM Intelligent Miner.

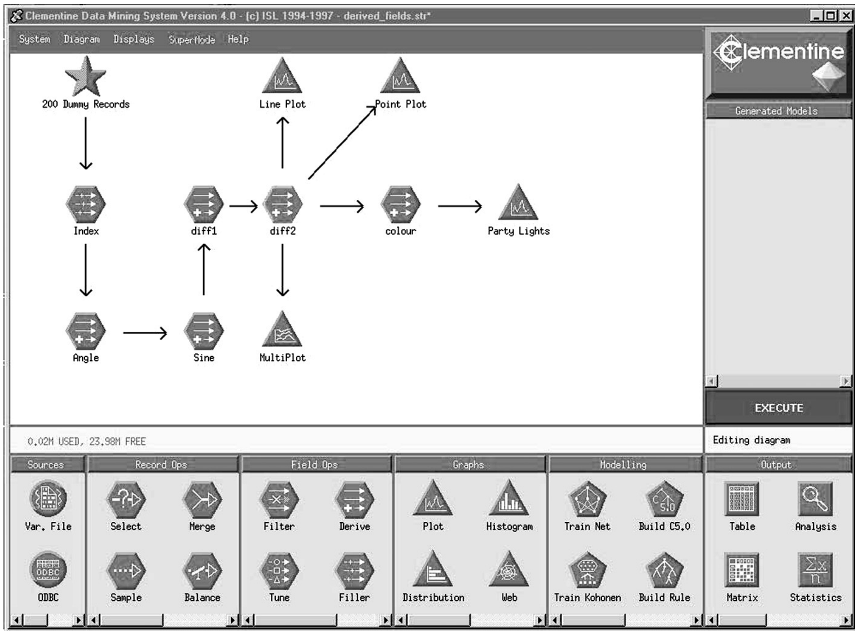
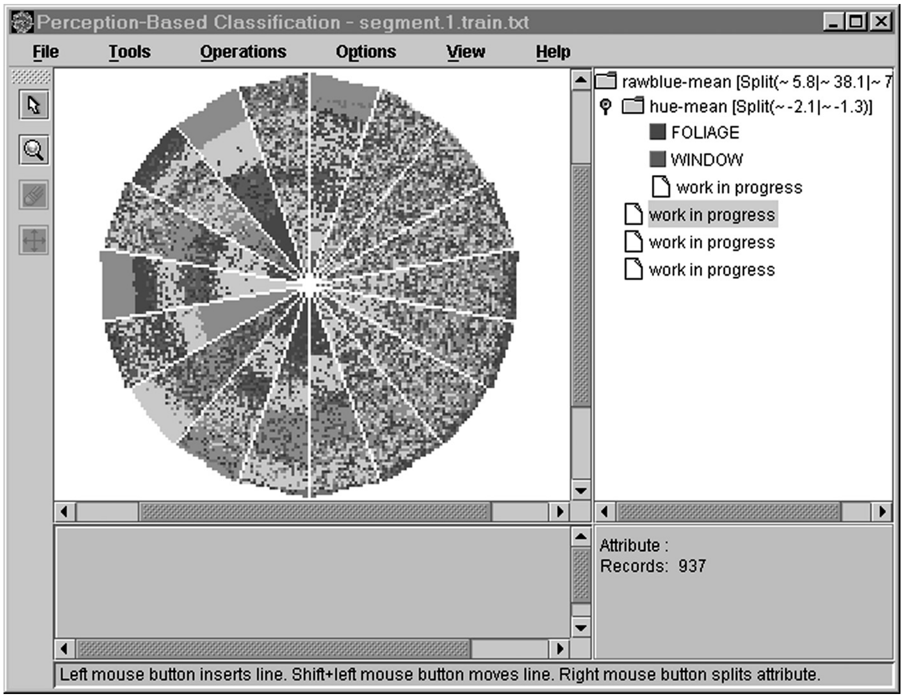


Figure 13.10 Visualization of data mining processes by Clementine.



Left mouse button inserts line. Shift+left mouse button moves line. Right mouse button splits attribute.

Figure 13.11 Perception-based classification, an interactive visual mining approach.

relaxing than visual mining. Therefore, audio data mining is an interesting complement to visual mining.

13.3 Data Mining Applications

In this book, we have studied principles and methods for mining relational data, data warehouses, and complex data types. Because data mining is a relatively young discipline with wide and diverse applications, there is still a nontrivial gap between general principles of data mining and application-specific, effective data mining tools. In this section, we examine several application domains, as listed in Figure 13.12. We discuss how customized data mining methods and tools should be developed for such applications.

13.3.1 Data Mining for Financial Data Analysis

Most banks and financial institutions offer a wide variety of banking, investment, and credit services (the latter include business, mortgage, and automobile loans and credit cards). Some also offer insurance and stock investment services.

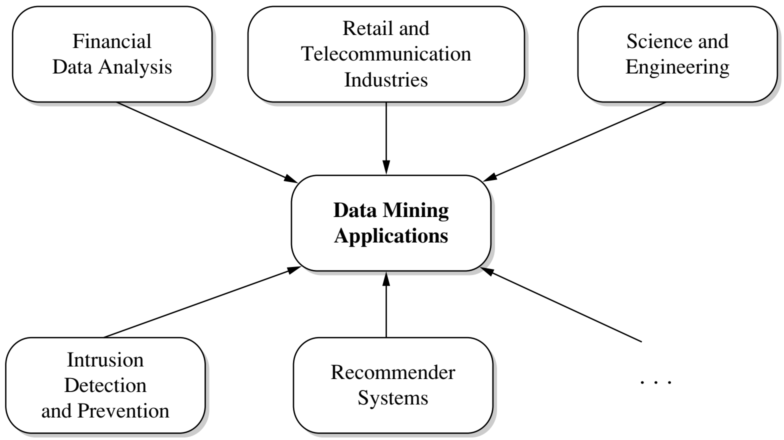


Figure 13.12 Common data mining application domains.

Financial data collected in the banking and financial industry are often relatively complete, reliable, and of high quality, which facilitates systematic data analysis and data mining. Here we present a few typical cases.

- **Design and construction of data warehouses for multidimensional data analysis and data mining:** Like many other applications, data warehouses need to be constructed for banking and financial data. Multidimensional data analysis methods should be used to analyze the general properties of such data. For example, a company's financial officer may want to view the debt and revenue changes by month, region, and sector, and other factors, along with maximum, minimum, total, average, trend, deviation, and other statistical information. Data warehouses, data cubes (including advanced data cube concepts such as multifeature, discovery-driven, regression, and prediction data cubes), characterization and class comparisons, clustering, and outlier analysis will all play important roles in financial data analysis and mining.
- **Loan payment prediction and customer credit policy analysis:** Loan payment prediction and customer credit analysis are critical to the business of a bank. Many factors can strongly or weakly influence loan payment performance and customer credit rating. Data mining methods, such as attribute selection and attribute relevance ranking, may help identify important factors and eliminate irrelevant ones. For example, factors related to the risk of loan payments include loan-to-value ratio, term of the loan, debt ratio (total amount of monthly debt versus total monthly income), payment-to-income ratio, customer income level, education level, residence region, and credit history. Analysis of the customer payment history may find that, say, payment-to-income ratio is a dominant factor, while education level and debt ratio are not. The bank may then decide to adjust its loan-granting policy so

as to grant loans to those customers whose applications were previously denied but whose profiles show relatively low risks according to the critical factor analysis.

- **Classification and clustering of customers for targeted marketing:** Classification and clustering methods can be used for customer group identification and targeted marketing. For example, we can use classification to identify the most crucial factors that may influence a customer's decision regarding banking. Customers with similar behaviors regarding loan payments may be identified by multidimensional clustering techniques. These can help identify customer groups, associate a new customer with an appropriate customer group, and facilitate targeted marketing.
- **Detection of money laundering and other financial crimes:** To detect money laundering and other financial crimes, it is important to integrate information from multiple, heterogeneous databases (e.g., bank transaction databases and federal or state crime history databases), as long as they are potentially related to the study. Multiple data analysis tools can then be used to detect unusual patterns, such as large amounts of cash flow at certain periods, by certain groups of customers. Useful tools include data visualization tools (to display transaction activities using graphs by time and by groups of customers), linkage and information network analysis tools (to identify links among different customers and activities), classification tools (to filter unrelated attributes and rank the highly related ones), clustering tools (to group different cases), outlier analysis tools (to detect unusual amounts of fund transfers or other activities), and sequential pattern analysis tools (to characterize unusual access sequences). These tools may identify important relationships and patterns of activities and help investigators focus on suspicious cases for further detailed examination.

13.3.2 Data Mining for Retail and Telecommunication Industries

The retail industry is a well-fit application area for data mining, since it collects huge amounts of data on sales, customer shopping history, goods transportation, consumption, and service. The quantity of data collected continues to expand rapidly, especially due to the increasing availability, ease, and popularity of business conducted on the Web, or **e-commerce**. Today, most major chain stores also have web sites where customers can make purchases online. Some businesses, such as Amazon.com (*www.amazon.com*), exist solely online, without any brick-and-mortar (i.e., physical) store locations. Retail data provide a rich source for data mining.

Retail data mining can help identify customer buying behaviors, discover customer shopping patterns and trends, improve the quality of customer service, achieve better customer retention and satisfaction, enhance goods consumption ratios, design more effective goods transportation and distribution policies, and reduce the cost of business.

A few examples of data mining in the retail industry are outlined as follows:

- **Design and construction of data warehouses:** Because retail data cover a wide spectrum (including sales, customers, employees, goods transportation, consumption, and services), there can be many ways to design a data warehouse for this industry. The levels of detail to include can vary substantially. The outcome of preliminary data mining exercises can be used to help guide the design and development of data warehouse structures. This involves deciding which dimensions and levels to include and what preprocessing to perform to facilitate effective data mining.

- **Multidimensional analysis of sales, customers, products, time, and region:** The retail industry requires timely information regarding customer needs, product sales, trends, and fashions, as well as the quality, cost, profit, and service of commodities. It is therefore important to provide powerful multidimensional analysis and visualization tools, including the construction of sophisticated data cubes according to the needs of data analysis. The *advanced data cube structures* introduced in Chapter 5 are useful in retail data analysis because they facilitate analysis on multidimensional aggregates with complex conditions.
- **Analysis of the effectiveness of sales campaigns:** The retail industry conducts sales campaigns using advertisements, coupons, and various kinds of discounts and bonuses to promote products and attract customers. Careful analysis of the effectiveness of sales campaigns can help improve company profits. Multidimensional analysis can be used for this purpose by comparing the amount of sales and the number of transactions containing the sales items during the sales period versus those containing the same items before or after the sales campaign. Moreover, association analysis may disclose which items are likely to be purchased together with the items on sale, especially in comparison with the sales before or after the campaign.
- **Customer retention—analysis of customer loyalty:** We can use customer loyalty card information to register sequences of purchases of particular customers. Customer loyalty and purchase trends can be analyzed systematically. Goods purchased at different periods by the same customers can be grouped into sequences. Sequential pattern mining can then be used to investigate changes in customer consumption or loyalty and suggest adjustments on the pricing and variety of goods to help retain customers and attract new ones.
- **Product recommendation and cross-referencing of items:** By mining associations from sales records, we may discover that a customer who buys a digital camera is likely to buy another set of items. Such information can be used to form product recommendations. *Collaborative recommender systems* (Section 13.3.5) use data mining techniques to make personalized product recommendations during live customer transactions, based on the opinions of other customers. Product recommendations can also be advertised on sales receipts, in weekly flyers, or on the Web to help improve customer service, aid customers in selecting items, and increase sales. Similarly, information, such as "hot items this week" or attractive deals, can be displayed together with the associative information to promote sales.
- **Fraudulent analysis and the identification of unusual patterns:** Fraudulent activity costs the retail industry millions of dollars per year. It is important to (1) identify potentially fraudulent users and their atypical usage patterns; (2) detect attempts to gain fraudulent entry or unauthorized access to individual and organizational

accounts; and (3) discover unusual patterns that may need special attention. Many of these patterns can be discovered by multidimensional analysis, cluster analysis, and outlier analysis.

As another industry that handles huge amounts of data, the **telecommunication industry** has quickly evolved from offering local and long-distance telephone services to providing many other comprehensive communication services. These include cellular phone, smart phone, Internet access, email, text messages, images, computer and web data transmissions, and other data traffic. The integration of telecommunication, computer network, Internet, and numerous other means of communication and computing has been under way, changing the face of telecommunications and computing. This has created a great demand for data mining to help understand business dynamics, identify telecommunication patterns, catch fraudulent activities, make better use of resources, and improve service quality.

Data mining tasks in telecommunications share many similarities with those in the retail industry. Common tasks include constructing large-scale data warehouses, performing multidimensional visualization, OLAP, and in-depth analysis of trends, customer patterns, and sequential patterns. Such tasks contribute to business improvements, cost reduction, customer retention, fraud analysis, and sharpening the edges of competition. There are many data mining tasks for which customized data mining tools for telecommunication have been flourishing and are expected to play increasingly important roles in business.

Data mining has been popularly used in many other industries, such as *insurance, manufacturing, and health care*, as well as for the *analysis of governmental and institutional administration data*. Although each industry has its own characteristic data sets and application demands, they share many common principles and methodologies. Therefore, through effective mining in one industry, we may gain experience and methodologies that can be transferred to other industrial applications.

13.3.3 Data Mining in Science and Engineering

In the past, many scientific data analysis tasks tended to handle relatively small and homogeneous data sets. Such data were typically analyzed using a "*formulate hypothesis, build model, and evaluate results*" paradigm. In these cases, statistical techniques were typically employed for their analysis (see Section 13.2.1). Massive data collection and storage technologies have recently changed the landscape of scientific data analysis. Today, scientific data can be amassed at much higher speeds and lower costs. This has resulted in the accumulation of huge volumes of high-dimensional data, stream data, and heterogenous data, containing rich spatial and temporal information. Consequently, scientific applications are shifting from the "*hypothesize-and-test*" paradigm toward a "*collect and store data, mine for new hypotheses, confirm with data or experimentation*" process. This shift brings about new challenges for data mining.

Vast amounts of data have been collected from scientific domains (including geosciences, astronomy, meteorology, geology, and biological sciences) using sophisticated telescopes, multispectral high-resolution remote satellite sensors, global positioning systems, and new generations of biological data collection and analysis technologies. Large data sets are also being generated due to fast numeric simulations in various fields such as climate and ecosystem modeling, chemical engineering, fluid dynamics, and structural mechanics. Here we look at some of the challenges brought about by emerging scientific applications of data mining.

- **Data warehouses and data preprocessing**: Data preprocessing and data warehouses are critical for information exchange and data mining. Creating a warehouse often requires finding means for resolving inconsistent or incompatible data collected in multiple environments and at different time periods. This requires reconciling semantics, referencing systems, geometry, measurements, accuracy, and precision. Methods are needed for integrating data from heterogeneous sources and for identifying events.

  For instance, consider climate and ecosystem data, which are spatial and temporal and require cross-referencing geospatial data. A major problem in analyzing such data is that there are too many events in the spatial domain but too few in the temporal domain. For example, El Nino events occur only every four to seven years, and previous data on them might not have been collected as systematically as they are today. Methods are also needed for the efficient computation of sophisticated spatial aggregates and the handling of spatial-related data streams.

- **Mining complex data types**: Scientific data sets are heterogeneous in nature. They typically involve semi-structured and unstructured data, such as multimedia data and georeferenced stream data, as well as data with sophisticated, deeply hidden semantics (e.g., genomic and proteomic data). Robust and dedicated analysis methods are needed for handling spatiotemporal data, biological data, related concept hierarchies, and complex semantic relationships. For example, in bioinformatics, a research problem is to identify regulatory influences on genes. *Gene regulation* refers to how genes in a cell are switched on (or off) to determine the cell's functions. Different biological processes involve different sets of genes acting together in precisely regulated patterns. Thus, to understand a biological process we need to identify the participating genes and their regulators. This requires the development of sophisticated data mining methods to analyze large biological data sets for clues about regulatory influences on specific genes, by finding DNA segments ("regulatory sequences") mediating such influence.

- **Graph-based and network-based mining**: It is often difficult or impossible to model several physical phenomena and processes due to limitations of existing modeling approaches. Alternatively, labeled graphs and networks may be used to capture many of the spatial, topological, geometric, biological, and other relational characteristics present in scientific data sets. In graph or network modeling, each object to be mined is represented by a vertex in a graph, and edges between vertices represent relationships between objects. For example, graphs can be used to model chemical structures, biological pathways, and data generated by numeric simulations such as fluid-flow simulations. The success of graph or network modeling, however, depends on improvements in the scalability and efficiency of many graph-based data mining tasks such as classification, frequent pattern mining, and clustering.

- **Visualization tools and domain-specific knowledge**: High-level graphical user interfaces and visualization tools are required for scientific data mining systems. These should be integrated with existing domain-specific data and information systems to guide researchers and general users in searching for patterns, interpreting and visualizing discovered patterns, and using discovered knowledge in their decision making.

Data mining in engineering shares many similarities with data mining in science. Both practices often collect massive amounts of data, and require data preprocessing, data warehousing, and scalable mining of complex types of data. Both typically use visualization and make good use of graphs and networks. Moreover, many engineering processes need real-time responses, and so mining data streams in real time often becomes a critical component.

Massive amounts of human communication data pour into our daily life. Such communication exists in many forms, including news, blogs, articles, web pages, online discussions, product reviews, twitters, messages, advertisements, and communications, both on the Web and in various kinds of social networks. Hence, **data mining in social science and social studies** has become increasingly popular. Moreover, user or reader feedback regarding products, speeches, and articles can be analyzed to deduce general opinions and sentiments on the views of those in society. The analysis results can be used to predict trends, improve work, and help in decision making.

Computer science generates unique kinds of data. For example, computer programs can be long, and their execution often generates huge-size traces. Computer networks can have complex structures and the network flows can be dynamic and massive. Sensor networks may generate large amounts of data with varied reliability. Computer systems and databases can suffer from various kinds of attacks, and their system/data accessing may raise security and privacy concerns. These unique kinds of data provide fertile land for data mining.

Data mining in computer science can be used to help monitor system status, improve system performance, isolate software bugs, detect software plagiarism, analyze computer system faults, uncover network intrusions, and recognize system malfunctions. Data mining for software and system engineering can operate on static or dynamic (i.e., stream-based) data, depending on whether the system dumps traces beforehand for postanalysis or if it must react in real time to handle online data.

Various methods have been developed in this domain, which integrate and extend methods from machine learning, data mining, software/system engineering, pattern recognition, and statistics. Data mining in computer science is an active and rich domain for data miners because of its unique challenges. It requires the further development of sophisticated, scalable, and real-time data mining and software/system engineering methods.

13.3.4 Data Mining for Intrusion Detection and Prevention

The security of our computer systems and data is at continual risk. The extensive growth of the Internet and the increasing availability of tools and tricks for intruding and attacking networks have prompted **intrusion detection and prevention** to become a critical component of networked systems. An intrusion can be defined as any set of actions that threaten the integrity, confidentiality, or availability of a network resource (e.g., user accounts, file systems, system kernels, and so on). Intrusion detection systems and intrusion prevention systems both monitor network traffic and/or system executions for malicious activities. However, the former produces reports whereas the latter is placed in-line and is able to actively prevent/block intrusions that are detected. The main functions of an intrusion prevention system are to identify malicious activity, log information about said activity, attempt to block/stop activity, and report activity.

The majority of intrusion detection and prevention systems use either *signature-based detection* or *anomaly-based detection.*

- **Signature-based detection**: This method of detection utilizes *signatures*, which are attack patterns that are preconfigured and predetermined by domain experts. A signature-based intrusion prevention system monitors the network traffic for matches to these signatures. Once a match is found, the intrusion detection system will report the anomaly and an intrusion prevention system will take additional appropriate actions. Note that since the systems are usually quite dynamic, the signatures need to be updated laboriously whenever new software versions arrive or changes in network configuration or other situations occur. Another drawback is that such a detection mechanism can only identify cases that match the signatures. That is, it is unable to detect new or previously unknown intrusion tricks.
- **Anomaly-based detection**: This method builds models of normal network behavior (called *profiles*) that are then used to detect new patterns that significantly deviate from the profiles. Such deviations may represent actual intrusions or simply be new behaviors that need to be added to the profiles. The main advantage of anomaly detection is that it may detect novel intrusions that have not yet been observed. Typically, a human analyst must sort through the deviations to ascertain which represent real intrusions. A limiting factor of anomaly detection is the high percentage of false positives. New patterns of intrusion can be added to the set of signatures to enhance signature-based detection.

Data mining methods can help an intrusion detection and prevention system to enhance its performance in various ways as follows.

- **New data mining algorithms for intrusion detection**: Data mining algorithms can be used for both signature-based and anomaly-based detection. In signature-based detection, training data are labeled as either "normal" or "intrusion." A classifier can then be derived to detect known intrusions. Research in this area has included the application of classification algorithms, association rule mining, and cost-sensitive modeling. Anomaly-based detection builds models of normal behavior and automatically detects significant deviations from it. Methods include the application of clustering, outlier analysis, and classification algorithms and statistical approaches. The techniques used must be efficient and scalable, and capable of handling network data of high volume, dimensionality, and heterogeneity.

- **Association, correlation, and discriminative pattern analyses help select and build discriminative classifiers**: Association, correlation, and discriminative pattern mining can be applied to find relationships between system attributes describing the network data. Such information can provide insight regarding the selection of useful attributes for intrusion detection. New attributes derived from aggregated data may also be helpful such as summary counts of traffic matching a particular pattern.
- **Analysis of stream data**: Due to the transient and dynamic nature of intrusions and malicious attacks, it is crucial to perform intrusion detection in the data stream environment. Moreover, an event may be normal on its own, but considered malicious if viewed as part of a sequence of events. Thus, it is necessary to study what sequences of events are frequently encountered together, find sequential patterns, and identify outliers. Other data mining methods for finding evolving clusters and building dynamic classification models in data streams are also necessary for real-time intrusion detection.
- **Distributed data mining**: Intrusions can be launched from several different locations and targeted to many different destinations. Distributed data mining methods may be used to analyze network data from several network locations to detect these distributed attacks.
- **Visualization and querying tools**: Visualization tools should be available for viewing any anomalous patterns detected. Such tools may include features for viewing associations, discriminative patterns, clusters, and outliers. Intrusion detection systems should also have a graphical user interface that allows security analysts to pose queries regarding the network data or intrusion detection results.

In summary, computer systems are at continual risk of breaks in security. Data mining technology can be used to develop strong intrusion detection and prevention systems, which may employ signature-based or anomaly-based detection.

13.3.5 Data Mining and Recommender Systems

Today's consumers are faced with millions of goods and services when shopping online. **Recommender systems** help consumers by making product recommendations that are likely to be of interest to the user such as books, CDs, movies, restaurants, online news articles, and other services. Recommender systems may use either a *content-based* approach, a *collaborative* approach, or a *hybrid* approach that combines both content-based and collaborative methods.

The **content-based approach** recommends items that are similar to items the user preferred or queried in the past. It relies on product features and textual item descriptions. The **collaborative approach** (or *collaborative filtering approach*) may consider a user's social environment. It recommends items based on the opinions of other customers who have similar tastes or preferences as the user. Recommender systems use a broad range of techniques from information retrieval, statistics, machine learning, and data mining to search for similarities among items and customer preferences. Consider Example 13.1.

Example 13.1 **Scenarios of using a recommender system.** Suppose that you visit the web site of an online bookstore (e.g., Amazon) with the intention of purchasing a book that you have been wanting to read. You type in the name of the book. This is not the first time you have visited the web site. You have browsed through it before and even made purchases from it last Christmas. The web store remembers your previous visits, having stored click stream information and information regarding your past purchases. The system displays the description and price of the book you have just specified. It compares your interests with other customers having similar interests and recommends additional book titles, saying *"Customers who bought the book you have specified also bought these other titles as well."* From surveying the list, you see another title that sparks your interest and decide to purchase that one as well.

Now suppose you go to another online store with the intention of purchasing a digital camera. The system suggests additional items to consider based on previously mined sequential patterns, such as *"Customers who buy this kind of digital camera are likely to buy a particular brand of printer, memory card, or photo editing software within three months."* You decide to buy just the camera, without any additional items. A week later, you receive coupons from the store regarding the additional items. ■

An advantage of recommender systems is that they provide *personalization* for customers of e-commerce, promoting one-to-one marketing. Amazon, a pioneer in the use of collaborative recommender systems, offers "a personalized store for every customer" as part of their marketing strategy. Personalization can benefit both consumers and the company involved. By having more accurate models of their customers, companies gain a better understanding of customer needs. Serving these needs can result in greater success regarding cross-selling of related products, upselling, product affinities, one-to-one promotions, larger baskets, and customer retention.

The recommendation problem considers a set, C, of users and a set, S, of items. Let u be a utility function that measures the usefulness of an item, s, to a user, c. The utility is commonly represented by a rating and is initially defined only for items previously rated by users. For example, when joining a movie recommendation system, users are typically asked to rate several movies. The space $C \times S$ of all possible users and items is huge. The recommendation system should be able to extrapolate from known to unknown ratings so as to predict item–user combinations. Items with the highest predicted rating/utility for a user are recommended to that user.

"How is the utility of an item estimated for a user?" In content-based methods, it is estimated based on the utilities assigned by the same user to other items that are similar. Many such systems focus on recommending items containing textual information, such as web sites, articles, and news messages. They look for commonalities among items. For movies, they may look for similar genres, directors, or actors. For articles, they may look for similar terms. Content-based methods are rooted in information theory. They make use of keywords (describing the items) and user profiles that contain information about users' tastes and needs. Such profiles may be obtained explicitly (e.g., through questionnaires) or learned from users' transactional behavior over time.

A collaborative recommender system tries to predict the utility of items for a user, u, based on items previously rated by other users who are similar to u. For example, when recommending books, a collaborative recommender system tries to find other users who have a history of agreeing with u (e.g., they tend to buy similar books, or give similar ratings for books). Collaborative recommender systems can be either memory (or heuristic) based or model based.

Memory-based methods essentially use heuristics to make rating predictions based on the entire collection of items previously rated by users. That is, the unknown rating of an item–user combination can be estimated as an aggregate of ratings of the most similar users for the same item. Typically, a k-nearest-neighbor approach is used, that is, we find the k other users (or neighbors) that are most similar to our target user, u. Various approaches can be used to compute the similarity between users. The most popular approaches use either Pearson's correlation coefficient (Section 3.3.2) or cosine similarity (Section 2.4.7). A weighted aggregate can be used, which adjusts for the fact that different users may use the rating scale differently. Model-based collaborative recommender systems use a collection of ratings to learn a model, which is then used to make rating predictions. For example, probabilistic models, clustering (which finds clusters of like-minded customers), Bayesian networks, and other machine learning techniques have been used.

Recommender systems face major challenges such as scalability and ensuring quality recommendations to the consumer. For example, regarding scalability, collaborative recommender systems must be able to search through millions of potential neighbors in real time. If the site is using browsing patterns as indications of product preference, it may have thousands of data points for some of its customers. Ensuring quality recommendations is essential to gain consumers' trust. If consumers follow a system recommendation but then do not end up liking the product, they are less likely to use the recommender system again.

As with classification systems, recommender systems can make two types of errors: false negatives and false positives. Here, *false negatives* are products that the system fails to recommend, although the consumer would like them. *False positives* are products that are recommended, but which the consumer does not like. False positives are less desirable because they can annoy or anger consumers. Content-based recommender systems are limited by the features used to describe the items they recommend.

Another challenge for both content-based and collaborative recommender systems is how to deal with new users for which a buying history is not yet available.

Hybrid approaches integrate both content-based and collaborative methods to achieve further improved recommendations. The Netflix Prize was an open competition held by an online DVD-rental service, with a payout of $1,000,000 for the best recommender algorithm to predict user ratings for films, based on previous ratings. The competition and other studies have shown that the predictive accuracy of a recommender system can be substantially improved when blending multiple predictors, especially by using an ensemble of many substantially different methods, rather than refining a single technique.

Collaborative recommender systems are a form of **intelligent query answering**, which consists of analyzing the intent of a query and providing generalized, neighborhood, or associated information relevant to the query. For example, rather than simply returning the book description and price in response to a customer's query, returning additional information that is related to the query but that was not explicitly asked for (e.g., book evaluation comments, recommendations of other books, or sales statistics) provides an intelligent answer to the same query.

13.4 Data Mining and Society

For most of us, data mining is part of our daily lives, although we may often be unaware of its presence. Section 13.4.1 looks at several examples of "ubiquitous and invisible" data mining, affecting everyday things from the products stocked at our local supermarket, to the ads we see while surfing the Internet, to crime prevention. Data mining can offer the individual many benefits by improving customer service and satisfaction as well as lifestyle, in general. However, it also has serious implications regarding one's right to privacy and data security. These issues are the topic of Section 13.4.2.

13.4.1 Ubiquitous and Invisible Data Mining

Data mining is present in many aspects of our daily lives, whether we realize it or not. It affects how we shop, work, and search for information, and can even influence our leisure time, health, and well-being. In this section, we look at examples of such **ubiquitous** (or ever-present) **data mining**. Several of these examples also represent **invisible data mining**, in which "smart" software, such as search engines, customer-adaptive web services (e.g., using recommender algorithms), "intelligent" database systems, email managers, ticket masters, and so on, incorporates data mining into its functional components, often unbeknownst to the user.

From grocery stores that print personalized coupons on customer receipts to online stores that recommend additional items based on customer interests, data mining has innovatively influenced what we buy, the way we shop, and our experience while shopping. One example is Wal-Mart, which has hundreds of millions of customers visiting its tens of thousands of stores every week. Wal-Mart allows suppliers to access data on their products and perform analyses using data mining software. This allows suppliers to identify customer buying patterns at different stores, control inventory and product placement, and identify new merchandizing opportunities. All of these affect which items (and how many) end up on the stores' shelves—something to think about the next time you wander through the aisles at Wal-Mart.

Data mining has shaped the online shopping experience. Many shoppers routinely turn to online stores to purchase books, music, movies, and toys. Recommender systems, discussed in Section 13.3.5, offer personalized product recommendations based on the opinions of other customers. Amazon.com was at the forefront of using such a personalized, data mining–based approach as a marketing strategy. It has observed that in traditional brick-and-mortar stores, the hardest part is getting the customer into the store. Once the customer is there, he or she is likely to buy something, since the cost of going to another store is high. Therefore, the marketing for brick-and-mortar stores tends to emphasize drawing customers in, rather than the actual in-store customer experience. This is in contrast to online stores, where customers can "walk out" and enter another online store with just a click of the mouse. Amazon.com capitalized on this difference, offering a "personalized store for every customer." They use several data mining techniques to identify customer's likes and make reliable recommendations.

While we are on the topic of shopping, suppose you have been doing a lot of buying with your credit cards. Nowadays, it is not unusual to receive a phone call from one's credit card company regarding suspicious or unusual patterns of spending. Credit card companies use data mining to detect fraudulent usage, saving billions of dollars a year.

Many companies increasingly use data mining for **customer relationship management (CRM)**, which helps provide more customized, personal service addressing individual customer's needs, in lieu of mass marketing. By studying browsing and purchasing patterns on web stores, companies can tailor advertisements and promotions to customer profiles, so that customers are less likely to be annoyed with unwanted mass mailings or junk mail. These actions can result in substantial cost savings for companies. The customers further benefit in that they are more likely to be notified of offers that are actually of interest, resulting in less waste of personal time and greater satisfaction.

Data mining has greatly influenced the ways in which people use computers, search for information, and work. Once you get on the Internet, for example, you decide to check your email. Unbeknownst to you, several annoying emails have already been deleted, thanks to a spam filter that uses classification algorithms to recognize spam. After processing your email, you go to Google (*www.google.com*), which provides access to information from billions of web pages indexed on its server. Google is one of the most popular and widely used Internet search engines. Using Google to search for information has become a way of life for many people.

Google is so popular that it has even become a new verb in the English language, meaning "to search for (something) on the Internet using the Google search engine or, by extension, any comprehensive search engine."[1] You decide to type in some keywords

[1] *http://open-dictionary.com.*

for a topic of interest. Google returns a list of web sites on your topic, mined, indexed, and organized by a set of data mining algorithms including PageRank. Moreover, if you type "Boston New York," Google will show you bus and train schedules from Boston to New York; however, a minor change to "Boston Paris" will lead to flight schedules from Boston to Paris. Such smart offerings of information or services are likely based on the frequent patterns mined from the click streams of many previous queries.

While you are viewing the results of your Google query, various ads pop up relating to your query. Google's strategy of tailoring advertising to match the user's interests is one of the typical services being explored by every Internet search provider. This also makes you happier, because you are less likely to be pestered with irrelevant ads.

Data mining is omnipresent, as can be seen from these daily-encountered examples. We could go on and on with such scenarios. In many cases, data mining is invisible, as users may be unaware that they are examining results returned by data mining or that their clicks are actually fed as new data into some data mining functions. For data mining to become further improved and accepted as a technology, continuing research and development are needed in the many areas mentioned as challenges throughout this book. These include efficiency and scalability, increased user interaction, incorporation of background knowledge and visualization techniques, effective methods for finding interesting patterns, improved handling of complex data types and stream data, real-time data mining, web mining, and so on. In addition, the *integration* of data mining into existing business and scientific technologies, to provide domain-specific data mining tools, will further contribute to the advancement of the technology. The success of data mining solutions tailored for e-commerce applications, as opposed to generic data mining systems, is an example.

13.4.2 Privacy, Security, and Social Impacts of Data Mining

With more and more information accessible in electronic forms and available on the Web, and with increasingly powerful data mining tools being developed and put into use, there are increasing concerns that data mining may pose a threat to our privacy and data security. However, it is important to note that many data mining applications do not even touch personal data. Prominent examples include applications involving natural resources, the prediction of floods and droughts, meteorology, astronomy, geography, geology, biology, and other scientific and engineering data. Furthermore, most studies in data mining research focus on the development of scalable algorithms and do not involve personal data.

The focus of data mining technology is on the *discovery of general or statistically significant patterns*, not on specific information regarding individuals. In this sense, we believe that the real privacy concerns are with unconstrained access to individual records, especially access to privacy-sensitive information such as credit card transaction records, health-care records, personal financial records, biological traits, criminal/justice investigations, and ethnicity. For the data mining applications that do involve personal data, in many cases, simple methods such as removing sensitive IDs from data may protect the privacy of most individuals. Nevertheless, privacy concerns exist wherever *personally identifiable information* is collected and stored in digital form, and data mining programs are able to access such data, even during data preparation.

Improper or nonexistent disclosure control can be the root cause of privacy issues. To handle such concerns, numerous data security-enhancing techniques have been developed. In addition, there has been a great deal of recent effort on developing *privacy-preserving* data mining methods. In this section, we look at some of the advances in protecting privacy and data security in data mining.

"What can we do to secure the privacy of individuals while collecting and mining data?" Many **data security–enhancing techniques** have been developed to help protect data. Databases can employ a *multilevel security model* to classify and restrict data according to various security levels, with users permitted access to only their authorized level. It has been shown, however, that users executing specific queries at their authorized security level can still infer more sensitive information, and that a similar possibility can occur through data mining. *Encryption* is another technique in which individual data items may be encoded. This may involve *blind signatures* (which build on public key encryption), *biometric encryption* (e.g., where the image of a person's iris or fingerprint is used to encode his or her personal information), and *anonymous databases* (which permit the consolidation of various databases but limit access to personal information only to those who need to know; personal information is encrypted and stored at different locations). Intrusion detection is another active area of research that helps protect the privacy of personal data.

Privacy-preserving data mining is an area of data mining research in response to privacy protection in data mining. It is also known as *privacy-enhanced* or *privacy-sensitive* data mining. It deals with obtaining valid data mining results without disclosing the underlying sensitive data values. Most privacy-preserving data mining methods use some form of transformation on the data to perform privacy preservation. Typically, such methods reduce the granularity of representation to preserve privacy. For example, they may generalize the data from individual customers to customer groups. This reduction in granularity causes loss of information and possibly of the usefulness of the data mining results. This is the natural trade-off between information loss and privacy. Privacy-preserving data mining methods can be classified into the following categories.

- **Randomization methods**: These methods add noise to the data to mask some attribute values of records. The noise added should be sufficiently large so that individual record values, especially sensitive ones, cannot be recovered. However, it should be added skillfully so that the final results of data mining are basically preserved. Techniques are designed to derive aggregate distributions from the perturbed data. Subsequently, data mining techniques can be developed to work with these aggregate distributions.
- **The *k*-anonymity and *l*-diversity methods**: Both of these methods alter individual records so that they cannot be uniquely identified. In the *k-anonymity method*, the granularity of data representation is reduced sufficiently so that any given record maps onto at least *k* other records in the data. It uses techniques like generalization and suppression. The *k*-anonymity method is weak in that, if there is a homogeneity

of sensitive values within a group, then those values may be inferred for the altered records. The *l-diversity model* was designed to handle this weakness by enforcing intragroup diversity of sensitive values to ensure anonymization. The goal is to make it sufficiently difficult for adversaries to use combinations of record attributes to exactly identify individual records.

- **Distributed privacy preservation**: Large data sets could be partitioned and distributed either *horizontally* (i.e., the data sets are partitioned into different subsets of records and distributed across multiple sites) or *vertically* (i.e., the data sets are partitioned and distributed by their attributes), or even in a combination of both. While the individual sites may not want to share their entire data sets, they may consent to limited information sharing with the use of a variety of protocols. The overall effect of such methods is to maintain privacy for each individual object, while deriving aggregate results over all of the data.
- **Downgrading the effectiveness of data mining results**: In many cases, even though the data may not be available, the output of data mining (e.g, association rules and classification models) may result in violations of privacy. The solution could be to downgrade the effectiveness of data mining by either modifying data or mining results, such as hiding some association rules or slightly distorting some classification models.

Recently, researchers proposed new ideas in privacy-preserving data mining such as the notion of **differential privacy**. The general idea is that, for any two data sets that are close to one another (i.e., that differ only on a tiny data set such as a single element), a given *differentially private algorithm* will behave approximately the same on both data sets. This definition gives a strong guarantee that the presence or absence of a tiny data set (e.g., representing an individual) will not affect the final output of the query significantly. Based on this notion, a set of differential privacy-preserving data mining algorithms have been developed. Research in this direction is ongoing. We expect more powerful privacy-preserving data publishing and data mining algorithms in the near future.

Like any other technology, data mining can be misused. However, we must not lose sight of all the benefits that data mining research can bring, ranging from insights gained from medical and scientific applications to increased customer satisfaction by helping companies better suit their clients' needs. We expect that computer scientists, policy experts, and counterterrorism experts will continue to work with social scientists, lawyers, companies, and consumers to take responsibility in building solutions to ensure data privacy protection and security. In this way, we may continue to reap the benefits of data mining in terms of time and money savings and the discovery of new knowledge.

13.5 Data Mining Trends

The diversity of data, data mining tasks, and data mining approaches poses many challenging research issues in data mining. The development of efficient and effective data mining methods, systems and services, and interactive and integrated data mining environments is a key area of study. The use of data mining techniques to solve large or sophisticated application problems is an important task for data mining researchers and data mining system and application developers. This section describes some of the trends in data mining that reflect the pursuit of these challenges.

- **Application exploration:** Early data mining applications put a lot of effort into helping businesses gain a competitive edge. The exploration of data mining for businesses continues to expand as e-commerce and e-marketing have become mainstream in the retail industry. Data mining is increasingly used for the exploration of applications in other areas such as web and text analysis, financial analysis, industry, government, biomedicine, and science. Emerging application areas include data mining for counterterrorism and mobile (wireless) data mining. Because generic data mining systems may have limitations in dealing with application-specific problems, we may see a trend toward the development of more application-specific data mining systems and tools, as well as invisible data mining functions embedded in various kinds of services.
- **Scalable and interactive data mining methods:** In contrast with traditional data analysis methods, data mining must be able to handle huge amounts of data efficiently and, if possible, interactively. Because the amount of data being collected continues to increase rapidly, scalable algorithms for individual and integrated data mining functions become essential. One important direction toward improving the overall efficiency of the mining process while increasing user interaction is **constraint-based mining**. This provides users with added control by allowing the specification and use of constraints to guide data mining systems in their search for interesting patterns and knowledge.
- **Integration of data mining with search engines, database systems, data warehouse systems, and cloud computing systems:** Search engines, database systems, data warehouse systems, and cloud computing systems are mainstream information processing and computing systems. It is important to ensure that data mining serves as an essential data analysis component that can be smoothly integrated into such an information processing environment. A data mining subsystem/service should be tightly coupled with such systems as a seamless, unified framework or as an invisible function. This will ensure data availability, data mining portability, scalability, high performance, and an integrated information processing environment for multidimensional data analysis and exploration.
- **Mining social and information networks:** Mining social and information networks and link analysis are critical tasks because such networks are ubiquitous and complex. The development of scalable and effective knowledge discovery methods and applications for large numbers of network data is essential, as outlined in Section 13.1.2.
- **Mining spatiotemporal, moving-objects, and cyber-physical systems:** Cyber-physical systems as well as spatiotemporal data are mounting rapidly due to the

popular use of cellular phones, GPS, sensors, and other wireless equipment. As outlined in Section 13.1.3, there are many challenging research issues realizing real-time and effective knowledge discovery with such data.

- **Mining multimedia, text, and web data:** As outlined in Section 13.1.3, mining such kinds of data is a recent focus in data mining research. Great progress has been made, yet there are still many open issues to be solved.
- **Mining biological and biomedical data:** The unique combination of complexity, richness, size, and importance of biological and biomedical data warrants special attention in data mining. Mining DNA and protein sequences, mining high-dimensional microarray data, and biological pathway and network analysis are just a few topics in this field. Other areas of biological data mining research include mining biomedical literature, link analysis across heterogeneous biological data, and information integration of biological data by data mining.
- **Data mining with software engineering and system engineering:** Software programs and large computer systems have become increasingly bulky in size sophisticated in complexity, and tend to originate from the integration of multiple components developed by different implementation teams. This trend has made it an increasingly challenging task to ensure software robustness and reliability. The analysis of the executions of a buggy software program is essentially a data mining process—tracing the data generated during program executions may disclose important patterns and outliers that could lead to the eventual automated discovery of software bugs. We expect that the further development of data mining methodologies for software/system debugging will enhance software robustness and bring new vigor to software/system engineering.
- **Visual and audio data mining:** Visual and audio data mining is an effective way to integrate with humans' visual and audio systems and discover knowledge from huge amounts of data. A systematic development of such techniques will facilitate the promotion of human participation for effective and efficient data analysis.
- **Distributed data mining and real-time data stream mining:** Traditional data mining methods, designed to work at a centralized location, do not work well in many of the distributed computing environments present today (e.g., the Internet, intranets, local area networks, high-speed wireless networks, sensor networks, and cloud computing). Advances in distributed data mining methods are expected. Moreover, many applications involving stream data (e.g., e-commerce, Web mining, stock analysis, intrusion detection, mobile data mining, and data mining for counterterrorism) require dynamic data mining models to be built in real time. Additional research is needed in this direction.
- **Privacy protection and information security in data mining:** An abundance of personal or confidential information available in electronic forms, coupled with increasingly powerful data mining tools, poses a threat to data privacy and security. Growing interest in data mining for counterterrorism also adds to the concern.

Further development of privacy-preserving data mining methods is foreseen. The collaboration of technologists, social scientists, law experts, governments, and companies is needed to produce a rigorous privacy and security protection mechanism for data publishing and data mining.

With confidence, we look forward to the next generation of data mining technology and the further benefits that it will bring.

13.6 Summary

- Mining complex data types poses challenging issues, for which there are many dedicated lines of research and development. This chapter presents a high-level overview of **mining complex data types**, which includes *mining sequence data* such as time series, symbolic sequences, and biological sequences; *mining graphs and networks*; and mining other kinds of data, including *spatiotemporal and cyber-physical system data*, *multimedia, text and Web data*, and *data streams.*
- Several well-established **statistical methods** have been proposed for data analysis such as regression, generalized linear models, analysis of variance, mixed-effect models, factor analysis, discriminant analysis, survival analysis, and quality control. Full coverage of statistical data analysis methods is beyond the scope of this book. Interested readers are referred to the statistical literature cited in the bibliographic notes (Section 13.8).
- Researchers have been striving to build **theoretical foundations** for data mining. Several interesting proposals have appeared, based on data reduction, data compression, probability and statistics theory, microeconomic theory, and pattern discovery–based inductive databases.
- **Visual data mining** integrates data mining and data visualization to discover implicit and useful knowledge from large data sets. Visual data mining includes *data visualization*, *data mining result visualization*, *data mining process visualization,* and *interactive visual data mining.* **Audio data mining** uses audio signals to indicate data patterns or features of data mining results.
- Many customized data mining tools have been developed for **domain-specific applications**, including finance, the retail and telecommunication industries, science and engineering, intrusion detection and prevention, and recommender systems. Such application domain-based studies integrate domain-specific knowledge with data analysis techniques and provide mission-specific data mining solutions.
- **Ubiquitous data mining** is the constant presence of data mining in many aspects of our daily lives. It can influence how we shop, work, search for information, and use a computer, as well as our leisure time, health, and well-being. In **invisible data mining**, "smart" software, such as search engines, customer-adaptive web services

(e.g., using recommender algorithms), email managers, and so on, incorporates data mining into its functional components, often unbeknownst to the user.

- A major social concern of data mining is the issue of *privacy and data security*. **Privacy-preserving data mining** deals with obtaining valid data mining results without disclosing underlying sensitive values. Its goal is to ensure privacy protection and security while preserving the overall quality of data mining results.
- **Data mining trends** include further efforts toward the exploration of new application areas; improved scalable, interactive, and constraint-based mining methods; the integration of data mining with web service, database, warehousing, and cloud computing systems; and mining social and information networks. Other trends include the mining of spatiotemporal and cyber-physical system data, biological data, software/system engineering data, and multimedia and text data, in addition to web mining, distributed and real-time data stream mining, visual and audio mining, and privacy and security in data mining.

13.7 Exercises

13.1 Sequence data are ubiquitous and have diverse applications. This chapter presented a general overview of sequential pattern mining, sequence classification, sequence similarity search, trend analysis, biological sequence alignment, and modeling. However, we have not covered sequence clustering. Present an overview of methods for *sequence clustering.*

13.2 This chapter presented an overview of sequence pattern mining and graph pattern mining methods. Mining tree patterns and partial order patterns is also studied in research. *Summarize the methods for mining structured patterns*, including sequences, trees, graphs, and partial order relationships. Examine what kinds of structural pattern mining have not been covered in research. Propose applications that can be created for such new mining problems.

13.3 Many studies analyze homogeneous information networks (e.g., social networks consisting of friends linked with friends). However, many other applications involve *heterogeneous information networks* (i.e., networks linking multiple types of object such as research papers, conference, authors, and topics). What are the major differences between methodologies for mining heterogeneous information networks and methods for their homogeneous counterparts?

13.4 Research and describe a *data mining application* that was not presented in this chapter. Discuss how different forms of data mining can be used in the application.

13.5 Why is the establishment of *theoretical foundations* important for data mining? Name and describe the main theoretical foundations that have been proposed for data mining. Comment on how they each satisfy (or fail to satisfy) the requirements of an ideal theoretical framework for data mining.

13.6 (**Research project**) Building a theory of data mining requires setting up a *theoretical framework* so that the major data mining functions can be explained under this framework. Take one theory as an example (e.g., data compression theory) and examine how the major data mining functions fit into this framework. If some functions do not fit well into the current theoretical framework, can you propose a way to extend the framework to explain these functions?

13.7 There is a strong linkage between *statistical data analysis* and data mining. Some people think of data mining as automated and scalable methods for statistical data analysis. Do you agree or disagree with this perception? Present one statistical analysis method that can be automated and/or scaled up nicely by integration with current data mining methodology.

13.8 What are the differences between *visual data mining* and *data visualization*? Data visualization may suffer from the data abundance problem. For example, it is not easy to visually discover interesting properties of network connections if a social network is huge, with complex and dense connections. Propose a visualization method that may help people see through the network topology to the interesting features of a social network.

13.9 Propose a few implementation methods for *audio data mining*. Can we integrate audio and *visual data mining* to bring fun and power to data mining? Is it possible to develop some video data mining methods? State some scenarios and your solutions to make such integrated audiovisual mining effective.

13.10 General-purpose computers and domain-independent relational database systems have become a large market in the last several decades. However, many people feel that generic data mining systems will not prevail in the data mining market. What do you think? For data mining, should we focus our efforts on developing *domain-independent* data mining tools or on developing *domain-specific* data mining solutions? Present your reasoning.

13.11 What is a *recommender system*? In what ways does it differ from a customer or product-based clustering system? How does it differ from a typical classification or predictive modeling system? Outline one method of collaborative filtering. Discuss why it works and what its limitations are in practice.

13.12 Suppose that your local bank has a data mining system. The bank has been studying your debit card usage patterns. Noticing that you make many transactions at home renovation stores, the bank decides to contact you, offering information regarding their special loans for home improvements.

(a) Discuss how this may conflict with your right to *privacy*.

(b) Describe another situation in which you feel that data mining can infringe on your privacy.

(c) Describe a *privacy-preserving data mining* method that may allow the bank to perform customer pattern analysis without infringing on its customers' right to privacy.

(d) What are some examples where data mining could be used to help society? Can you think of ways it could be used that may be detrimental to society?

13.13 What are the major challenges faced in bringing data mining research to *market*? Illustrate one data mining research issue that, in your view, may have a strong impact on the market and on society. Discuss how to approach such a research issue.

13.14 Based on your view, what is the most *challenging research problem* in data mining? If you were given a number of years and a good number of researchers and implementors, what would your plan be to make good progress toward an effective solution to such a problem?

13.15 Based on your experience and knowledge, suggest a *new frontier* in data mining that was not mentioned in this chapter.

13.8 Bibliographic Notes

For mining complex data types, there are many research papers and books covering various themes. We list here some recent books and well-cited survey or research articles for references.

Time-series analysis has been studied in statistics and computer science communities for decades, with many textbooks such as Box, Jenkins, and Reinsel [BJR08]; Brockwell and Davis [BD02]; Chatfield [Cha03b]; Hamilton [Ham94]; and Shumway and Stoffer [SS05]. A fast subsequence matching method in time-series databases was presented by Faloutsos, Ranganathan, and Manolopoulos [FRM94]. Agrawal, Lin, Sawhney, and Shim [ALSS95] developed a method for fast **similarity search** in the presence of noise, scaling, and translation in time-series databases. Shasha and Zhu present an overview of the methods for high-performance discovery in time series [SZ04].

Sequential pattern mining methods have been studied by many researchers, including Agrawal and Srikant [AS95]; Zaki [Zak01]; Pei, Han, Mortazavi-Asl, et al. [PHM-A$^+$04]; and Yan, Han, and Afshar [YHA03]. The study on **sequence classification** includes Ji, Bailey, and Dong [JBD05] and Ye and Keogh [YK09], with a survey by Xing, Pei, and Keogh [XPK10]. Dong and Pei [DP07] provide an overview on **sequence data mining** methods.

Methods for **analysis of biological sequences** including **Markov chains** and **hidden Markov models** are introduced in many books or tutorials such as Waterman [Wat95]; Setubal and Meidanis [SM97]; Durbin, Eddy, Krogh, and Mitchison [DEKM98]; Baldi and Brunak [BB01]; Krane and Raymer [KR03]; Rabiner [Rab89]; Jones and Pevzner [JP04]; and Baxevanis and Ouellette [BO04]. Information about BLAST (see also Korf, Yandell, and Bedell [KYB03]) can be found at the NCBI web site *www.ncbi.nlm.nih.gov/BLAST/*.

Graph pattern mining has been studied extensively, including Holder, Cook, and Djoko [HCD94]; Inokuchi, Washio, and Motoda [IWM98]; Kuramochi and Karypis [KK01]; Yan and Han [YH02, YH03a]; Borgelt and Berthold [BB02]; Huan, Wang, Bandyopadhyay, et al. [HWB$^+$04]; and the Gaston tool by Nijssen and Kok [NK04].

There has been a great deal of research on **social and information network analysis**, including Newman [New10]; Easley and Kleinberg [EK10]; Yu, Han, and Faloutsos [YHF10]; Wasserman and Faust [WF94]; Watts [Wat03]; and Newman, Barabasi, and Watts [NBW06]. **Statistical modeling of networks** is studied popularly such as Albert and Barbasi [AB99]; Watts [Wat03]; Faloutsos, Faloutsos, and Faloutsos [FFF99]; Kumar, Raghavan, Rajagopalan, et al. [KRR$^+$00]; and Leskovec, Kleinberg, and Faloutsos [LKF05]. **Data cleaning, integration, and validation by information network analysis** was studied by many, including Bhattacharya and Getoor [BG04] and Yin, Han, and Yu [YHY07, YHY08].

Clustering, ranking, and classification in networks has been studied extensively, including in Brin and Page [BP98]; Chakrabarti, Dom, and Indyk [CDI98]; Kleinberg [Kle99]; Getoor, Friedman, Koller, and Taskar [GFKT01]; Newman and M. Girvan [NG04]; Yin, Han, Yang, and Yu [YHYY04]; Yin, Han, and Yu [YHY05]; Xu, Yuruk, Feng, and Schweiger [XYFS07]; Kulis, Basu, Dhillon, and Mooney [KBDM09]; Sun, Han, Zhao, et al. [SHZ$^+$09]; Neville, Gallaher, and Eliassi-Rad [NGE-R09]; and Ji, Sun, Danilevsky et al. [JSD$^+$10]. **Role discovery and link prediction in information networks** have been studied extensively as well, such as by Krebs [Kre02]; Kubica, Moore, and Schneider [KMS03]; Liben-Nowell and Kleinberg [L-NK03]; and Wang, Han, Jia, et al. [WHJ$^+$10].

Similarity search and OLAP in information networks has been studied by many, including Tian, Hankins, and Patel [THP08] and Chen, Yan, Zhu, et al. [CYZ$^+$08]. **Evolution of social and information networks** has been studied by many researchers, such as Chakrabarti, Kumar, and Tomkins [CKT06]; Chi, Song, Zhou, et al. [CSZ$^+$07]; Tang, Liu, Zhang, and Nazeri [TLZN08]; Xu, Zhang, Yu, and Long [XZYL08]; Kim and Han [KH09]; and Sun, Tang, and Han [STH$^+$10].

Spatial and spatiotemporal data mining has been studied extensively, with a collection of papers by Miller and Han [MH09], and was introduced in some textbooks, such as Shekhar and Chawla [SC03] and Hsu, Lee, and Wang [HLW07]. Spatial clustering algorithms have been studied extensively in Chapters 10 and 11 of this book. Research has been conducted on spatial warehouses and OLAP, such as by Stefanovic, Han, and Koperski [SHK00], and spatial and spatiotemporal data mining, such as by Koperski and Han [KH95]; Mamoulis, Cao, Kollios, Hadjieleftheriou, et al. [MCK$^+$04]; Tsoukatos and Gunopulos [TG01]; and Hadjieleftheriou, Kollios, Gunopulos, and Tsotras [HKGT03]. **Mining moving-object data** has been studied by many, such as Vlachos, Gunopulos, and Kollios [VGK02]; Tao, Faloutsos, Papadias, and Liu [TFPL04]; Li, Han, Kim, and Gonzalez [LHKG07]; Lee, Han, and Whang [LHW07]; and Li, Ding, Han, et al. [LDH$^+$10]. For the bibliography of temporal, spatial, and spatiotemporal data mining research, see a collection by Roddick, Hornsby, and Spiliopoulou [RHS01].

Multimedia data mining has deep roots in image processing and pattern recognition, which have been studied extensively in many textbooks, including Gonzalez and Woods [GW07]; Russ [Rus06]; Duda, Hart, and Stork [DHS01]; and Z. Zhang and R. Zhang [ZZ09]. Searching and mining of multimedia data has been studied by many (see, e.g., Fayyad and Smyth [FS93]; Faloutsos and Lin [FL95]; Natsev, Rastogi, and

Shim [NRS99]; and Zaïane, Han, and Zhu [ZHZ00]). An overview of image mining methods is given by Hsu, Lee, and Zhang [HLZ02].

Text data analysis has been studied extensively in information retrieval, with many textbooks and survey articles such as Croft, Metzler, and Strohman [CMS09]; S. Buttcher, C. Clarke, G. Cormack [BCC10]; Manning, Raghavan, and Schutze [MRS08]; Grossman and Frieder [GR04]; Baeza-Yates and Riberio-Neto [BYRN11]; Zhai [Zha08]; Feldman and Sanger [FS06]; Berry [Ber03]; and Weiss, Indurkhya, Zhang, and Damerau [WIZD04]. Text mining is a fast-developing field with numerous papers published in recent years, covering many topics such as topic models (e.g., Blei and Lafferty [BL09]); sentiment analysis (e.g., Pang and Lee [PL07]); and contextual text mining (e.g., Mei and Zhai [MZ06]).

Web mining is another focused theme, with books like Chakrabarti [Cha03a], Liu [Liu06], and Berry [Ber03]. Web mining has substantially improved search engines with a few influential milestone works, such as Brin and Page [BP98]; Kleinberg [Kle99]; Chakrabarti, Dom, Kumar, et al. [CDK+99]; and Kleinberg and Tomkins [KT99]. Numerous results have been generated since then, such as search log mining (e.g., Silvestri [Sil10]); blog mining (e.g., Mei, Liu, Su, and Zhai [MLSZ06]); and mining online forums (e.g., Cong, Wang, Lin, et al. [CWL+08]).

Books and surveys on stream data systems and stream data processing include Babu and Widom [BW01]; Babcock, Babu, Datar, et al. [BBD+02]; Muthukrishnan [Mut05]; and Aggarwal [Agg06].

Stream data mining research covers stream cube models (e.g., Chen, Dong, Han, et al. [CDH+02]), stream frequent pattern mining (e.g., Manku and Motwani [MM02] and Karp, Papadimitriou and Shenker [KPS03]), stream classification (e.g., Domingos and Hulten [DH00]; Wang, Fan, Yu, and Han [WFYH03]; Aggarwal, Han, Wang, and Yu [AHWY04b]), and stream clustering (e.g., Guha, Mishra, Motwani, and O'Callaghan [GMMO00] and Aggarwal, Han, Wang, and Yu [AHWY03]).

There are many books that discuss **data mining applications**. For financial data analysis and financial modeling, see, for example, Benninga [Ben08] and Higgins [Hig08]. For retail data mining and customer relationship management, see, for example, books by Berry and Linoff [BL04] and Berson, Smith, and Thearling [BST99]. For telecommunication-related data mining, see, for example, Horak [Hor08]. There are also books on scientific data analysis, such as Grossman, Kamath, Kegelmeyer, et al. [GKK+01] and Kamath [Kam09].

Issues in the **theoretical foundations of data mining** have been addressed by many researchers. For example, Mannila presents a summary of studies on the foundations of data mining in [Man00]. The data reduction view of data mining is summarized in *The New Jersey Data Reduction Report* by Barbará, DuMouchel, Faloutos, et al. [BDF+97]. The data compression view can be found in studies on the minimum description length principle, such as Grunwald and Rissanen [GR07].

The pattern discovery point of view of data mining is addressed in numerous machine learning and data mining studies, ranging from association mining, to decision tree induction, sequential pattern mining, clustering, and so on. The probability theory point of view is popular in the statistics and machine learning literature, such as Bayesian networks and hierarchical Bayesian models in Chapter 9, and probabilistic graph models (e.g., Koller and Friedman [KF09]). Kleinberg, Papadimitriou, and Raghavan [KPR98] present a microeconomic view, treating data mining as an optimization problem. Studies on the inductive database view include Imielinski and Mannila [IM96] and de Raedt, Guns, and Nijssen [RGN10].

Statistical methods for data analysis are described in many books, such as Hastie, Tibshirani, Friedman [HTF09]; Freedman, Pisani, and Purves [FPP07]; Devore [Dev03]; Kutner, Nachtsheim, Neter, and Li [KNNL04]; Dobson [Dob01]; Breiman, Friedman, Olshen, and Stone [BFOS84]; Pinheiro and Bates [PB00]; Johnson and Wichern [JW02b]; Huberty [Hub94]; Shumway and Stoffer [SS05]; and Miller [Mil98].

For **visual data mining**, popular books on the visual display of data and information include those by Tufte [Tuf90, Tuf97, Tuf01]. A summary of techniques for visualizing data is presented in Cleveland [Cle93]. A dedicated visual data mining book, *Visual Data Mining: Techniques and Tools for Data Visualization and Mining*, is by Soukup and Davidson [SD02]. The book *Information Visualization in Data Mining and Knowledge Discovery*, edited by Fayyad, Grinstein, and Wierse [FGW01], contains a collection of articles on visual data mining methods.

Ubiquitous and invisible data mining has been discussed in many texts including John [Joh99], and some articles in a book edited by Kargupta, Joshi, Sivakumar, and Yesha [KJSY04]. The book *Business @ the Speed of Thought: Succeeding in the Digital Economy* by Gates [Gat00] discusses e-commerce and customer relationship management, and provides an interesting perspective on data mining in the future. Mena [Men03] has an informative book on the use of data mining to detect and prevent crime. It covers many forms of criminal activities, ranging from fraud detection, money laundering, insurance crimes, identity crimes, and intrusion detection.

Data mining issues regarding **privacy and data security** are addressed popularly in literature. Books on privacy and security in data mining include Thuraisingham [Thu04]; Aggarwal and Yu [AY08]; Vaidya, Clifton, and Zhu [VCZ10]; and Fung, Wang, Fu, and Yu [FWFY10]. Research articles include Agrawal and Srikant [AS00]; Evfimievski, Srikant, Agrawal, and Gehrke [ESAG02]; and Vaidya and Clifton [VC03]. Differential privacy was introduced by Dwork [Dwo06] and studied by many such as Hay, Rastogi, Miklau, and Suciu [HRMS10].

There have been many discussions on **trends and research directions of data mining** in various forums. Several books are collections of articles on these issues such as Kargupta, Han, Yu, et al. [KHY$^+$08].

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