MATRICES

A matrix is a rectangular array of numbers, such as **A**. When $n = m$, **A** is a square matrix of order *n.*
Transposing all rows and columns in **A** is denoted as $\mathbf{A}^T$.
Matrices are a convenient notation heavily used in dealing with large systems of linear equations, which notably reduce in size to just **A X** = **B** or **X** = $\mathbf{A}^{-1}\mathbf{B}$, where $\mathbf{A}^{-1}$ denotes the inverse of matrix **A**.

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \cdots & \cdots & \cdots & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} b_1 & b_2 & \cdots & b_m \end{bmatrix}^T$$

$$\mathbf{X} = \begin{bmatrix} x_1 & x_2 & \cdots & x_m \end{bmatrix}^T$$

The main diagonal of a square matrix is the sequence of elements a_{11}, a_{22}, …, a_{nn} from upper left to lower right.

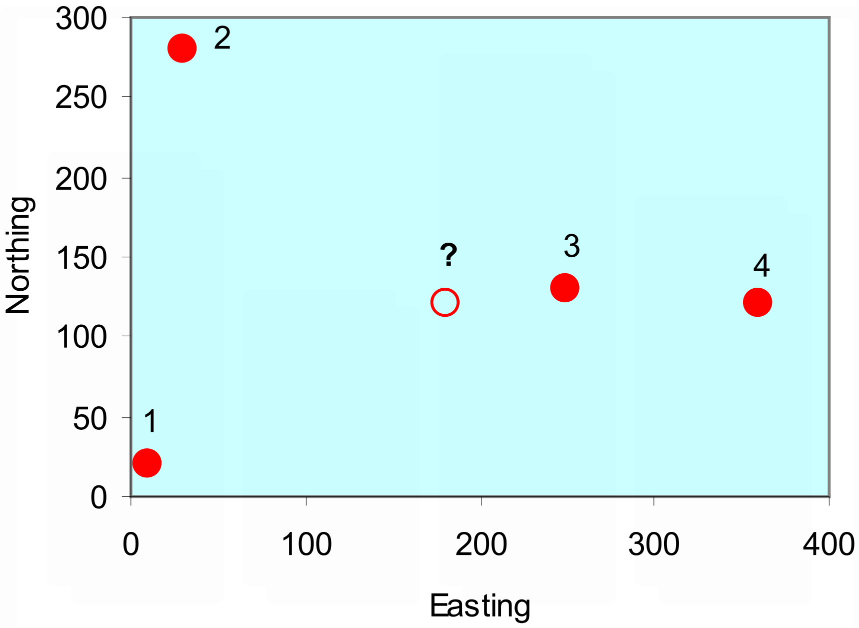
SIMPLE KRIGING MATRIX FORMULATION

$$\begin{bmatrix} \mathrm{Cov}(\mathbf{s}_1,\mathbf{s}_1) & \cdots & \mathrm{Cov}(\mathbf{s}_k,\mathbf{s}_1) \\ \vdots & \cdots & \vdots \\ \mathrm{Cov}(\mathbf{s}_1,\mathbf{s}_k) & \ldots & \mathrm{Cov}(\mathbf{s}_k,\mathbf{s}_k) \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{bmatrix} = \begin{bmatrix} \mathrm{Cov}(\mathbf{s}_0,\mathbf{s}_1) \\ \vdots \\ \mathrm{Cov}(\mathbf{s}_0,\mathbf{s}_K) \end{bmatrix}$$

$$Z_{SK}^*(\mathbf{s}_0) = m + \begin{bmatrix} Z(\mathbf{s}_1) - m \\ \vdots \\ Z(\mathbf{s}_k) - m \end{bmatrix}^T \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{bmatrix}$$

$$\sigma_{SK}^2(\mathbf{s}_0) = \mathrm{Cov}(\mathbf{s}_0,\mathbf{s}_0) - \begin{bmatrix} \mathrm{Cov}(\mathbf{s}_0,\mathbf{s}_1) \\ \vdots \\ \mathrm{Cov}(\mathbf{s}_0,\mathbf{s}_k) \end{bmatrix}^T \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{bmatrix}$$

EXERCISE



SAMPLE

Index	Easting	Northing	Attribute
1	10	20	40
2	30	280	130
3	250	130	90
4	360	120	160
?	180	120	

m=110

$$\mathrm{Cov}(\mathbf{h}) = 2000e^{-\mathbf{h}/250}$$

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EXERCISE

For the previous configuration, using simple kriging:

A. Discuss the weight values.
B. Find the estimate.
C. Compute the estimation variance.
D. Calculate the estimation weights.

A. CALCULATION OF WEIGHTS (1)

Distance matrix among observations:

$$\begin{bmatrix} 0 & & & \\ 260.8 & 0 & & \\ 264.0 & 266.3 & 0 & \\ 364.0 & 366.7 & 110.4 & 0 \end{bmatrix}$$

Distance from estimation location to each observation:

$$\begin{bmatrix} 197.2 & 219.3 & 70.7 & 180.0 \end{bmatrix}^T$$

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CALCULATION OF WEIGHTS (2)

Weights:

$$\begin{bmatrix} 2000 & & & \\ 704.8 & 2000 & & \\ 695.6 & 689.4 & 2000 & \\ 466.4 & 461.2 & 1285.8 & 2000 \end{bmatrix}^{-1} \begin{bmatrix} 908.7 \\ 831.8 \\ 1507.2 \\ 973.6 \end{bmatrix} = \begin{bmatrix} 0.185 \\ 0.128 \\ 0.646 \\ -0.001 \end{bmatrix}$$

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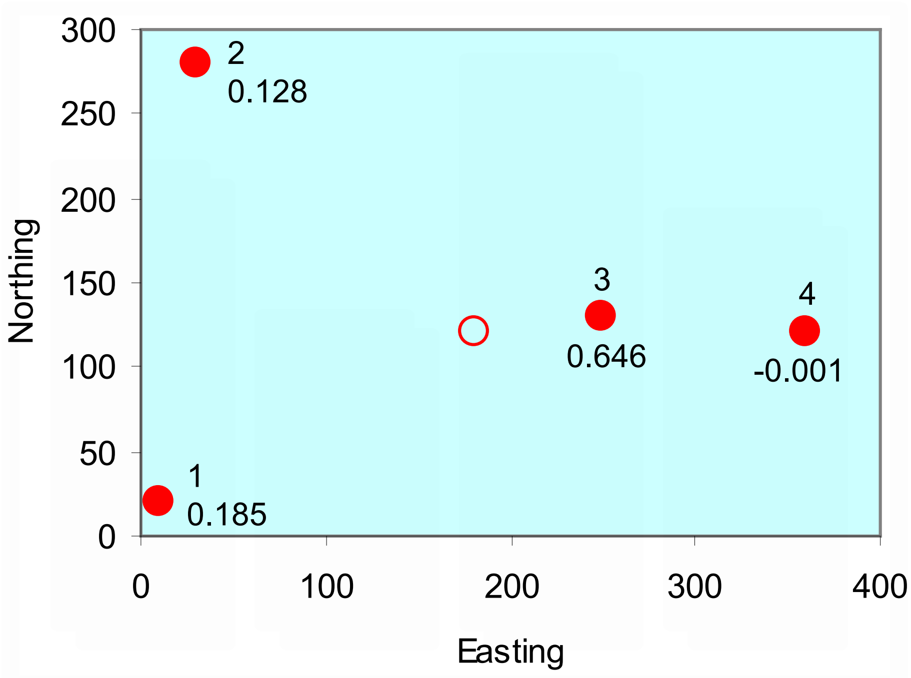
B. REMARKS



- Weight 4 is almost zero despite being closer to the estimation location than weight 1. This reduction known as screen effect is caused by the intermediate location of weight 3.
- Weight 4 is negative.
- Negative weights open the possibility to have estimates outside the extreme values of the data (nonconvexity).

C. ESTIMATE

$$z_{SK}^{*}(\mathbf{s}_0) = m + \begin{bmatrix} Z(\mathbf{s}_1) - m \\ \vdots \\ Z(\mathbf{s}_k) - m \end{bmatrix}^T \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{bmatrix}$$

$$z_{SK}^{*}(180,120) = 110 + \begin{bmatrix} 40 - 110 \\ 130 - 110 \\ 90 - 110 \\ 160 - 110 \end{bmatrix}^T \begin{bmatrix} 0.185 \\ 0.128 \\ 0.646 \\ -0.001 \end{bmatrix}$$

$$z_{SK}^{*}(180,120) = 86.7$$

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D. ESTIMATION VARIANCE

$$\sigma_{SK}^2(\mathbf{s}_0) = \mathrm{Cov}(\mathbf{s}_0, \mathbf{s}_0) - \begin{bmatrix} \mathrm{Cov}(\mathbf{s}_0, \mathbf{s}_1) \\ \vdots \\ \mathrm{Cov}(\mathbf{s}_0, \mathbf{s}_k) \end{bmatrix}^T \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{bmatrix}$$

$$\sigma_{SK}^2(180{,}120) = 2000 - \begin{bmatrix} 908.6 \\ 831.8 \\ 1507.2 \\ 973.6 \end{bmatrix}^T \begin{bmatrix} 0.185 \\ 0.128 \\ 0.646 \\ -0.001 \end{bmatrix}$$

$$\sigma_{SK}^2(180{,}120) = 752.9$$

PROPERTIES OF SIMPLE KRIGING

- Nonconvexity
- Screen effect
- Declustering
- Global unbiasedness
- Minimum mean-square-error optimality
- Exact interpolator
- When interpolation is exact, the error variance is 0
- Intolerance to duplicated sites
- The estimate is orthogonal to its error
- Independence to translation of Cartesian system

PROPERTIES OF SIMPLE KRIGING

- Independence of estimator to covariance scaling
- Scaling of covariance changes the estimation variance by same factor
- Estimation variance depends on data configuration
- Estimation variance does not depend directly on individual sample values
- If the weights sum up to 1, the estimator is independent of the value of the mean

MULTIGAUSSIAN KRIGING

- This is kriging of normal scores.
- The univariate marginal distribution of a multivariate normal distribution is normal, yet the converse is not true.
- Under multivariate normality, simple kriging is the best of all possible estimators, linear or nonlinear, biased or unbiased.
- Multivariate normality cannot be verified; at most, it cannot be rejected.
- Considering that the mean of normal scores is zero, if they are second order stationary, they provide a rare opportunity to apply simple kriging.
- Backtransformation of estimated normal scores outside the interval of variation for the normal scores of the data is highly uncertain.

9. ORDINARY KRIGING

BRILLIANT TRICK

One can rewrite the simple kriging estimator as

$$Z^*_{SK}(\mathbf{s}_0) = m\left(1 - \sum_{i=1}^{n} \lambda_i\right) + \sum_{i=1}^{n} \lambda_i Z(\mathbf{s}_i).$$

If the weights sum up to 1, then the estimator is independent of *m*, thus resulting in a more general formulation applicable to samples with constant, but unknown mean (no trend).

It can be proved than the constraint has the additional benefit of making the estimator unbiased.

Ordinary kriging was a first formulation of improved simple kriging. Simple kriging roots predate geostatistics. We will see that one can still find weights minimizing the mean square estimation error.

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ORDINARY KRIGING

The ordinary kriging estimator is:

$$Z^*_{OK}(\mathbf{s}_0) = \begin{cases} \sum_{i=1}^{k} \lambda_i Z(\mathbf{s}_i) \\ \sum_{i=1}^{k} \lambda_i = 1, \end{cases}$$

where:

$z^*_{OK}(\mathbf{s}_0)$ denotes estimation at geographic location $\mathbf{s}_0$;

$\mathbf{s}_i$ is the location of measurement i;

k denotes the number of observations to consider;

m is the mean of $Z(\mathbf{s})$; and

λ_i is a real weight.

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DERIVATION OF EQUATIONS

The whole purpose of ordinary kriging is to find optimal weights that minimize the mean square estimation error. The steps are the same as those required to formulate simple kriging:

A. Make necessary assumptions;
B. Find expression for estimation error variance;
C. Modify estimation error variance equation to have it in terms of covariances;
D. Out of all possible weights, find those that minimize the error variance.
E. Replace the optimal weights in the expression for error variance. This is the kriging variance.

A. STRONGER ASSUMPTIONS

1. The sample is a partial realization of a random function $Z(\mathbf{s})$, where **s** denotes spatial location.
2. $Z(\mathbf{s})$ is second order stationary, that is:

$$\mathrm{E}[Z(\mathbf{s})] = m$$

$$\mathrm{E}[(Z(\mathbf{s}) - m)(Z(\mathbf{s} + \mathbf{h}) - m)] = \mathrm{Cov}(\mathbf{h}),$$

where $\mathrm{E}[\cdot]$ denotes expected value, m is a scalar constant, and **h** is a vectorial distance.

As in simple kriging, the mean is still constant, but now it can be unknown.