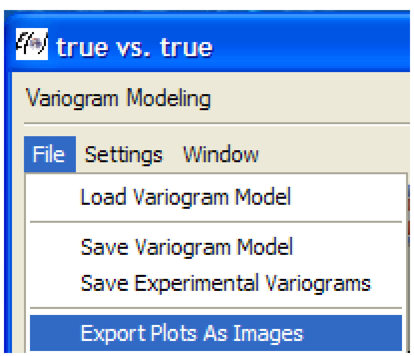
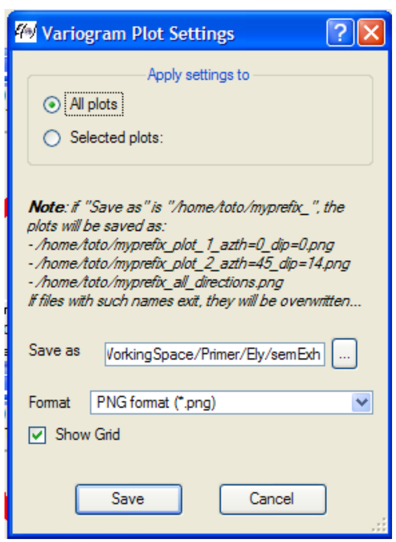
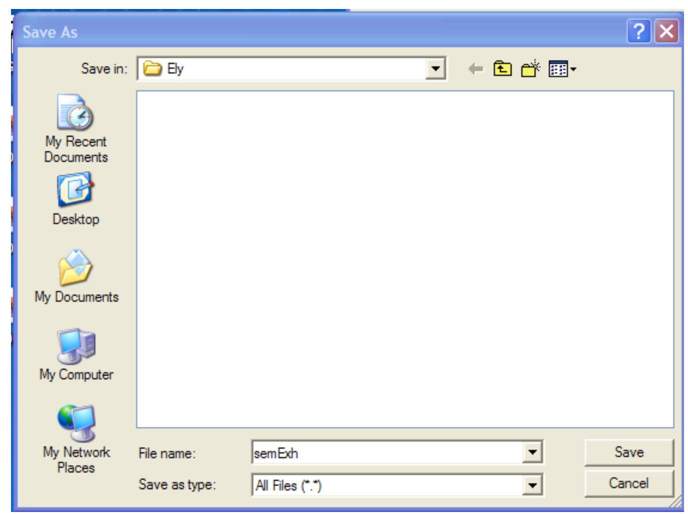
SAVING SEMIVARIOGRAMS

- Click on the <File> option of semivariogram modeling.
- Pick an option, for example, <Export Plot as Images>.
- Check <Show Grid> if it is desired to display it.
- Click on the three dots <…>.
- Select storage folder.
- Give generic name to semivariograms.
- Click on <Save> in both menus.



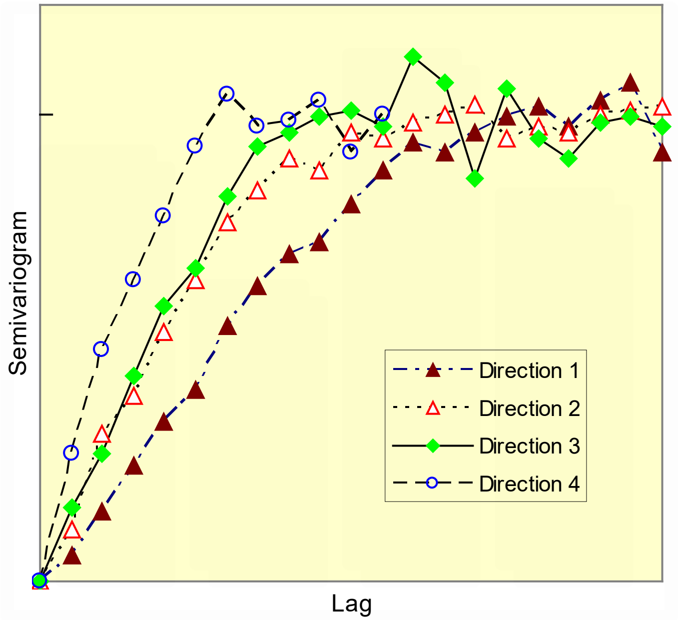




OTHER DIRECT APPLICATIONS

Direct applications of the semivariogram, not necessarily requiring to go through modeling, include:

- Detection of anisotropy by finding out if the semivariogram is different along different directions.

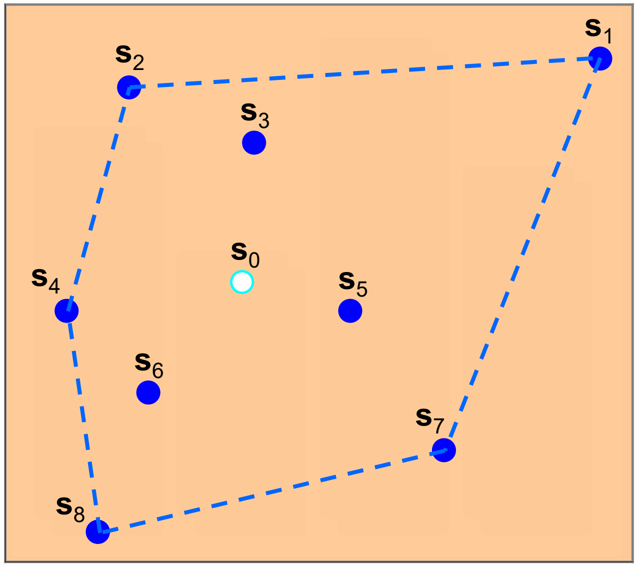


- Comparative studies of origins in the processes behind attributes based on the premise that different geneses lead to different semivariograms.
- Sampling design. In any direction, sampling interval should not exceed half the range.

8. SIMPLE KRIGING

KRIGING

Kriging is a form of generalized linear regression for the formulation of an optimal spatial estimator in a minimum mean-square-error sense.



Given some observations at locations $\mathbf{s}_i$, kriging provides an estimate and a standard error at locations, such as $\mathbf{s}_0$, typically not considered in the sampling.

In contrast to classical linear regression, kriging takes into account observation volume and stochastic dependence among data.

The method works best inside the convex hull determined by the peripheral data.

VARIANTS

There are several forms of kriging, each making different assumptions to adjust to different styles of attribute fluctuations.

- Simple kriging
- Ordinary kriging
- Universal kriging
- Lognormal kriging
- Indicator kriging

The last two types are simply any of the first three forms of kriging applied to transformed data as explained in chapter 6.

SIMPLE KRIGING

Simple kriging is the estimation of

$$z^*_{SK}(\mathbf{s}_0) = m + \sum_{i=1}^{n} \lambda_i \cdot (z(\mathbf{s}_i) - m),$$

where:

$z^*_{SK}(\mathbf{s}_0)$ is the estimator at geographical location $\mathbf{s}_0$;

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

n is the number of observations to consider;

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

λ_i is a real number, commonly referred to as weight.

NORMAL EQUATIONS

The originality of kriging is the use of weights, λ_i , such that they minimize the estimation error variance. Such weights turn out to be the solution of the following system of equations, called the normal system of equations:

$$\left.\begin{array}{rcl}
\sum_{i=1}^{k} \lambda_i \operatorname{Cov}\left(\mathbf{s}_i, \mathbf{s}_1\right) & = & \operatorname{Cov}\left(\mathbf{s}_0, \mathbf{s}_1\right) \\
\sum_{i=1}^{k} \lambda_i \operatorname{Cov}\left(\mathbf{s}_i, \mathbf{s}_2\right) & = & \operatorname{Cov}\left(\mathbf{s}_0, \mathbf{s}_2\right) \\
\cdots\cdots\cdots\cdots\cdots\cdots & \cdots & \cdots\cdots\cdots\cdots\cdots \\
\sum_{i=1}^{k} \lambda_i \operatorname{Cov}\left(\mathbf{s}_i, \mathbf{s}_k\right) & = & \operatorname{Cov}\left(\mathbf{s}_0, \mathbf{s}_k\right)
\end{array}\right\}$$

DERIVATION OF NORMAL EQUATIONS

The steps are:

A. Make necessary assumptions.
B. Calculate error variance.
C. Express error variance in terms of covariances.
D. Find the weights that minimize the error variance.
E. Calculate the minimum error variance.

A. 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, which implies:

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

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

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

3. Unique to simple kriging is the assumption that the mean is not only constant but known.

These assumptions make simple kriging the most restricted form of kriging.

The weakness of this simplicity is the same as with any simple model: limitation in its applicability or suboptimal results if its use is forced.

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B. ESTIMATION VARIANCE

By definition, the estimation variance is:

$$\sigma^2(\mathbf{s}_0) = \text{Var}\left[Z^*_{SK}(\mathbf{s}_0) - Z(\mathbf{s}_0)\right].$$

We know neither the random function $Z(\mathbf{s}_0)$ nor the estimator $Z^*_{SK}(\mathbf{s}_0)$, so we cannot directly calculate the variance of the difference.

The way to solve this conundrum is to transform the expression for the variance to have it in terms of quantities that we know.

C. ALGEBRAIC MANIPULATIONS (1)

The residual $Y(\mathbf{s})$ of a random function is the difference between the random function and its expected value. In this case:

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

Expressing this estimation variance in terms of the residuals, we have:

$$\sigma^2(\mathbf{s}_0) = \mathrm{Var}\left[\sum_{i=1}^{k} \lambda_i Y(\mathbf{s}_i) - Y(\mathbf{s}_0)\right] = \mathrm{Var}\left[\sum_{i=0}^{k} \lambda_i Y(\mathbf{s}_i)\right]$$

if one defines $\lambda_0 = -1$.

ALGEBRAIC MANIPULATIONS (2)

From the properties of the variance (pages 31 and 52):

$$\sigma^2(\mathbf{s}_0) = \mathrm{E}\left[\left\{\sum_{i=0}^{k} \lambda_i Y(\mathbf{s}_i)\right\}^2\right] - \left\{\mathrm{E}\left[\sum_{i=0}^{k} \lambda_i Y(\mathbf{s}_i)\right]\right\}^2.$$

Expanding the squares and introducing the expectations inside the summations:

$$\sigma^2(\mathbf{s}_0) = \sum_{i=0}^{k}\sum_{j=0}^{k} \lambda_i \lambda_j \,\mathrm{E}\left[Y(\mathbf{s}_i) Y(\mathbf{s}_j)\right] - \sum_{i=0}^{k}\sum_{j=0}^{k} \lambda_i \lambda_j \,\mathrm{E}\left[Y(\mathbf{s}_i)\right]\mathrm{E}\left[Y(\mathbf{s}_j)\right].$$

ALGEBRAIC MANIPULATIONS (3)

Grouping the terms by coefficients:

$$\sigma^2(\mathbf{s}_0) = \sum_{i=0}^{k}\sum_{j=0}^{k}\lambda_i\lambda_j\left\{\mathrm{E}\left[Y(\mathbf{s}_i)Y(\mathbf{s}_j)\right] - \mathrm{E}\left[Y(\mathbf{s}_i)\right]\mathrm{E}\left[Y(\mathbf{s}_j)\right]\right\}.$$

Backtransforming to the random function and expanding:

$$\sigma^2(\mathbf{s}_0) = \sum_{i=0}^{k}\sum_{j=0}^{k}\lambda_i\lambda_j\left\{\mathrm{E}\left[m^2 - mZ(\mathbf{s}_i) - mZ(\mathbf{s}_j) + Z(\mathbf{s}_i)Z(\mathbf{s}_j)\right]\right.$$
$$\left. - m^2 + m\mathrm{E}\left[Z(\mathbf{s}_i)\right] + m\mathrm{E}\left[Z(\mathbf{s}_j)\right] - \mathrm{E}\left[Z(\mathbf{s}_i)\right]\mathrm{E}\left[Z(\mathbf{s}_j)\right]\right\}.$$

Because of the cancelation of terms,

$$\sigma^2(\mathbf{s}_0) = \sum_{i=0}^{k}\sum_{j=0}^{k}\lambda_i\lambda_j\left\{\mathrm{E}\left[Z(\mathbf{s}_i)Z(\mathbf{s}_j)\right] - \mathrm{E}\left[Z(\mathbf{s}_i)\right]\mathrm{E}\left[Z(\mathbf{s}_j)\right]\right\},$$

ALGEBRAIC MANIPULATIONS (4)

which is the same as:

$$\sigma^2(\mathbf{s}_0) = \sum_{i=0}^{k} \sum_{j=0}^{k} \lambda_i \lambda_j \operatorname{Cov}(\mathbf{s}_i, \mathbf{s}_j).$$

Finally, remembering that $\lambda_0 = -1$:

$$\boxed{\begin{aligned}\sigma^2(\mathbf{s}_0) &= \operatorname{Cov}(\mathbf{s}_0, \mathbf{s}_0) - 2\sum_{i=1}^{k} \lambda_i \operatorname{Cov}(\mathbf{s}_0, \mathbf{s}_i) \\ &+ \sum_{i=1}^{k} \sum_{j=1}^{k} \lambda_i \lambda_j \operatorname{Cov}(\mathbf{s}_i, \mathbf{s}_j),\end{aligned}}$$

which is an expression in terms of covariance, a measurable property, hence a useful expression.

D. OPTIMAL WEIGHTS (1)

The expression for $\sigma^2(\mathbf{s}_0)$ is valid for any weights. Among the infinite weight combinations, we are interested in those that minimize the estimation variance associated with the estimator $Z^*_{SK}(\mathbf{s}_0)$.

The expression for $\sigma^2(\mathbf{s}_0)$ is quadratic in the unknowns, the weights. Under these circumstances, according to an operations research theorem, the necessary and sufficient condition to have a unique global nonnegative minimum is that the quadratic term must be larger than or equal to zero. This implies that the covariance function must be such that any combination, like the one in the general expression for $\sigma^2(\mathbf{s}_0)$, cannot be negative. In mathematics, such is the property of being positive definite. This is the condition a covariance model has to satisfy to be permissible.

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OPTIMAL WEIGHTS (2)

The optimal weights are those that make zero all partial derivatives of $\sigma^2(\mathbf{s}_0)$ with respect to the weights:

$$\frac{\partial \sigma^2(\mathbf{s}_0)}{\partial \lambda_j} = -2\,\mathrm{Cov}(\mathbf{s}_0, \mathbf{s}_j) + 2\sum_{i=1}^{k} \lambda_i\,\mathrm{Cov}(\mathbf{s}_i, \mathbf{s}_j) = 0$$

for all locations j, $j = 1, 2, \ldots, k$.

Cancellation of factor 2 and rearrangement give:

$$\boxed{\left.\begin{array}{lcl}
\sum_{i=1}^{k} \lambda_i\,\mathrm{Cov}(\mathbf{s}_i, \mathbf{s}_1) & = & \mathrm{Cov}(\mathbf{s}_0, \mathbf{s}_1) \\
\sum_{i=1}^{k} \lambda_i\,\mathrm{Cov}(\mathbf{s}_i, \mathbf{s}_2) & = & \mathrm{Cov}(\mathbf{s}_0, \mathbf{s}_2) \\
\cdots\cdots\cdots\cdots\cdots & \cdots & \cdots\cdots\cdots\cdots \\
\sum_{i=1}^{k} \lambda_i\,\mathrm{Cov}(\mathbf{s}_i, \mathbf{s}_k) & = & \mathrm{Cov}(\mathbf{s}_0, \mathbf{s}_k)
\end{array}\right\}}$$

E. OPTIMAL ESTIMATION VARIANCE

Multiplying each optimality condition by λ_i and adding them together, we have a new optimality relationship:

$$\sum_{i=1}^{k} \lambda_i \sum_{j=1}^{k} \lambda_j \operatorname{Cov}(\mathbf{s}_i, \mathbf{s}_j) = \sum_{i=1}^{k} \lambda_i \operatorname{Cov}(\mathbf{s}_0, \mathbf{s}_i).$$

Introducing λ_i under the second summation and replacing the resulting double summation in the general expression for $\sigma^2(\mathbf{s}_0)$:

$$\boxed{\sigma_{SK}^2(\mathbf{s}_0) = \operatorname{Cov}(\mathbf{s}_0, \mathbf{s}_0) - \sum_{i=1}^{k} \lambda_i \operatorname{Cov}(\mathbf{s}_0, \mathbf{s}_i).}$$

SUMMARY

Simple kriging normal equations for optimal weights λ_i:

$$\left.\begin{array}{lcl}\sum_{i=1}^{k}\lambda_i \operatorname{Cov}(\mathbf{s}_i,\mathbf{s}_1) & = & \operatorname{Cov}(\mathbf{s}_0,\mathbf{s}_1)\\ \sum_{i=1}^{k}\lambda_i \operatorname{Cov}(\mathbf{s}_i,\mathbf{s}_2) & = & \operatorname{Cov}(\mathbf{s}_0,\mathbf{s}_2)\\ \cdots\cdots\cdots\cdots & \cdots & \cdots\cdots\cdots\\ \sum_{i=1}^{k}\lambda_i \operatorname{Cov}(\mathbf{s}_i,\mathbf{s}_k) & = & \operatorname{Cov}(\mathbf{s}_0,\mathbf{s}_k)\end{array}\right\}$$

Simple kriging estimation:

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

Simple kriging mean-square-error variance:

$$\sigma_{SK}^{2}(\mathbf{s}_0) = \operatorname{Cov}(\mathbf{s}_0,\mathbf{s}_0) - \sum_{i=1}^{k}\lambda_i \operatorname{Cov}(\mathbf{s}_0,\mathbf{s}_i)$$