WEAKER ASSUMPTIONS

The following is a set of slightly weaker assumptions, in the sense that they do not require that the variance be finite.

1. The sample is a partial realization of a random function $Z(\mathbf{s})$, where **s** denotes spatial location.
2. $Z(\mathbf{s})$ honors the intrinsic hypothesis, meaning that:

$$\mathrm{E}[Z(\mathbf{s})] = m$$
$$\mathrm{Var}[Z(\mathbf{s}) - Z(\mathbf{s}+\mathbf{h})] = 2\gamma(\mathbf{h}),$$

where $\gamma(\mathbf{h})$ is the semivariogram.

The mean must be constant, but because it will not enter into the calculations, it can be unknown.

B. ESTIMATION VARIANCE

The estimation variance is the error variance:

$$\sigma^2(\mathbf{s}_0) = \mathrm{Var}\left[Z^*_{OK}(\mathbf{s}_0) - Z(\mathbf{s}_0)\right],$$

where $Z(\mathbf{s}_0)$ is the random function at the estimation location $\mathbf{s}_0$ and $Z^*_{OK}(\mathbf{s}_0)$ is the ordinary kriging estimator.

We know neither of these; thus, it is not possible to calculate $\sigma^2(\mathbf{s}_0)$. The way out is to transform the expression for the variance to have it in terms of quantities that we can calculate. This will require even more laborious algebraic manipulations than for simple kriging. Nothing comes for free!

LEMMA 1 (1)

Let $Z(\mathbf{s}_i)$ be a random variable of a continuous random function. Then for any coefficient λ_i:

$$\mathrm{E}\left[\left\{\sum_{i=1}^{k}\lambda_i Z(\mathbf{s}_i)\right\}^2\right] = \sum_{i=1}^{k}\sum_{j=1}^{k}\lambda_i\lambda_j\,\mathrm{E}\left[Z(\mathbf{s}_i)Z(\mathbf{s}_j)\right].$$

Proof:

One can regard $\lambda_i\lambda_j$ as a new constant and $Z(\mathbf{s}_i)Z(\mathbf{s}_j)$ as a new variable.

LEMMA 1 (2)

Then, by the distributive and commutative properties of the expectation:

$$\mathrm{E}\left[\left\{\sum_{i=1}^{k}\lambda_i Z(\mathbf{s}_i)\right\}^2\right] = \lambda_1\lambda_i\sum_{i=1}^{k}\mathrm{E}[Z(\mathbf{s}_1)Z(\mathbf{s}_i)]$$

$$+\lambda_2\lambda_i\sum_{i=1}^{k}\mathrm{E}[Z(\mathbf{s}_2)Z(\mathbf{s}_i)]+\ldots+\lambda_k\lambda_i\sum_{i=1}^{k}\mathrm{E}[Z(\mathbf{s}_k)Z(\mathbf{s}_i)]$$

and the proof follows by condensing the expression using a second summation index.

LEMMA 2 (1)

Let $Z(\mathbf{s}_i)$ be a random variable of a continuous random function. Then for any coefficient λ_i:

$$\mathrm{Var}\left[\left\{\sum_{i=1}^{k}\lambda_i Z(\mathbf{s}_i)\right\}^2\right]=\sum_{i=1}^{k}\sum_{j=1}^{k}\lambda_i\lambda_j\,\mathrm{Cov}\left[\mathbf{s}_i,\mathbf{s}_j\right].$$

Proof:

By the definition of variance (pages 31 and 52):

$$\mathrm{Var}\left[\sum_{i=i}^{k}\lambda_i Z(\mathbf{s}_i)\right]=\mathrm{E}\left[\left\{\sum_{i=1}^{k}\lambda_i Z(\mathbf{s}_i)\right\}^2\right]-\left\{\mathrm{E}\left[\sum_{i=1}^{k}\lambda_i Z(\mathbf{s}_i)\right]\right\}^2.$$

LEMMA 2 (2)

In the right side, by Lemma 1 and expanding second the term:

$$\mathrm{Var}\left[\sum_{i=1}^{k}\lambda_i Z(\mathbf{s}_i)\right]=\sum_{i=1}^{k}\sum_{j=1}^{k}\lambda_i\lambda_j\,\mathrm{E}\left[Z(\mathbf{s}_i)Z(\mathbf{s}_j)\right]$$

$$-\sum_{i=1}^{k}\sum_{j=1}^{k}\lambda_i\lambda_j\,\mathrm{E}\left[Z(\mathbf{s}_i)\right]\mathrm{E}\left[Z(\mathbf{s}_j)\right].$$

Factoring,

$$\mathrm{Var}\left[\sum_{i=1}^{k}\lambda_i Z(\mathbf{s}_i)\right]=\sum_{i=1}^{k}\sum_{j=1}^{k}\lambda_i\lambda_j\left\{\mathrm{E}\left[Z(\mathbf{s}_i)Z(\mathbf{s}_j)\right]\right.$$

$$\left.-\mathrm{E}\left[Z(\mathbf{s}_i)\right]\mathrm{E}\left[Z(\mathbf{s}_j)\right]\right\}.$$

The fact that the difference is equal to the covariance of $Z(\mathbf{s}_i)$ and $Z(\mathbf{s}_j)$ proves the lemma.

LEMMA 3 (1)

Let $Z(\mathbf{s})$ be an intrinsic random function. Then:

$$\gamma(\mathbf{s}_i - \mathbf{s}_j) = \gamma(\mathbf{s}_i - \mathbf{s}) + \gamma(\mathbf{s}_j - \mathbf{s}) - \mathrm{Cov}(\mathbf{s}_i - \mathbf{s}, \mathbf{s}_j - \mathbf{s}).$$

Proof:

By the stationarity assumption:

$$\gamma(\mathbf{s}_i - \mathbf{s}_j) = \frac{1}{2}\mathrm{E}\left[\{Z(\mathbf{s}_i) - Z(\mathbf{s}_j)\}^2\right],$$

which does not change by adding and subtracting a third variate

$$\gamma(\mathbf{s}_i - \mathbf{s}_j) = \frac{1}{2}\mathrm{E}\left[\{\{Z(\mathbf{s}_i) - Z(\mathbf{s})\} - \{Z(\mathbf{s}_j) - Z(\mathbf{s})\}\}^2\right].$$

LEMMA 3 (2)

Expanding:

$$\gamma(\mathbf{s}_i - \mathbf{s}_j) = \frac{1}{2}\mathrm{E}\left[\{Z(\mathbf{s}_i) - Z(\mathbf{s})\}^2\right] + \frac{1}{2}\mathrm{E}\left[\{Z(\mathbf{s}_j) - Z(\mathbf{s})\}^2\right]$$
$$- \mathrm{E}\left[Z(\mathbf{s}_i) - Z(\mathbf{s}), Z(\mathbf{s}_j) - Z(\mathbf{s})\right],$$

and again, by the stationarity assumption:

$$\gamma(\mathbf{s}_i - \mathbf{s}_j) = \gamma(\mathbf{s}_i - \mathbf{s}) + \gamma(\mathbf{s}_j - \mathbf{s})$$
$$- \mathrm{E}\left[Z(\mathbf{s}_i) - Z(\mathbf{s}), Z(\mathbf{s}_j) - Z(\mathbf{s})\right].$$

The proof follows from the definition of the covariance because of the special fact that the mean of the differences is zero because the mean is constant.

C. NEW ERROR VARIANCE EXPRESSION (1)

Replacing the estimator by its definition in the expression for the error variance:

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

because $\sum_{i=1}^{k} \lambda_i = 1$. From Lemma 2,

$$\sigma^2(\mathbf{s}_0) = \sum_{i=1}^{k} \sum_{j=1}^{k} \lambda_i \lambda_j \,\mathrm{Cov}\left(\mathbf{s}_i - \mathbf{s}_0, \mathbf{s}_j - \mathbf{s}_0\right),$$

which, by Lemma 3, is:

$$\sigma^2(\mathbf{s}_0) = \sum_{i=1}^{k} \sum_{j=1}^{k} \lambda_i \lambda_j \left\{\gamma(\mathbf{s}_i - \mathbf{s}_0) + \gamma(\mathbf{s}_j - \mathbf{s}_0) - \gamma(\mathbf{s}_i - \mathbf{s}_j)\right\}.$$

NEW ERROR VARIANCE EXPRESSION (2)

Expanding, because of the constraint $\sum_{i=1}^{k} \lambda_i = 1$:

$$\sigma^2(\mathbf{s}_0) = \sum_{i=1}^{k} \lambda_i \gamma(\mathbf{s}_i - \mathbf{s}_0) + \sum_{j=1}^{k} \lambda_j \gamma(\mathbf{s}_j - \mathbf{s}_0)$$

$$- \sum_{i=1}^{k} \sum_{j=1}^{k} \lambda_i \lambda_j \gamma(\mathbf{s}_i - \mathbf{s}_j).$$

The first two terms in the right-hand side of the equation are the same, thus:

$$\boxed{\sigma^2(\mathbf{s}_0) = 2\sum_{i=1}^{k} \lambda_i \gamma(\mathbf{s}_i - \mathbf{s}_0) - \sum_{i=1}^{k} \sum_{j=1}^{k} \lambda_i \lambda_j \gamma(\mathbf{s}_i - \mathbf{s}_j).}$$

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D. OPTIMAL WEIGHTS

The expression for $\sigma^2(\mathbf{s}_0)$ is quadratic in the unknowns, the weights. In such a case, the necessary and sufficient condition to have a unique global minimum is that the quadratic term must be equal to or larger than zero, which implies that the semivariogram must be negative definite. Thus, we need to employ only permissible models.

The expression for $\sigma^2(\mathbf{s}_0)$ is valid for any weights. Among the infinite weight combinations, we are interested in those minimizing the estimation variance associated with the estimator $Z^*_{OK}(\mathbf{s}_0)$. This is a constrained operations research problem, best solved by the Lagrange method of multipliers.

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LAGRANGE METHOD

The Lagrange method of multipliers is a procedure for the optimization of a function of several variables $f(y_1, y_2, \ldots, y_n)$ constrained by $\phi_1, \phi_2, \ldots, \phi_m$.

The solution is found by equating to 0 the n partial derivatives of an unconstrained auxiliary function

$$f(y_1, y_2, \ldots, y_n) + \sum_{i=1}^{m} \mu_i \phi_i$$

with respect to all y_i, regarding the Lagrange multipliers, μ_i, as constants.

The resulting n equations plus the original m constraints provide a system of equations from which the unknown y_i and the auxiliary variables, μ_i, can be calculated.

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TRIVIAL LAGRANGE EXAMPLE

To find the maximum area of a rectangle whose perimeter is the given value p, it is necessary to find the maximum value of the product of the sides $a \cdot b$, subject to the constraint $2a + 2b - p = 0$.

The auxiliary function is in this case

$$u = ab + \mu(2a + 2b - p),$$

which after differentiation with respect to the unknowns a and b gives

$$\left.\begin{aligned} a + 2\mu &= 0 \\ b + 2\mu &= 0 \\ 2a + 2b &= p \end{aligned}\right\}$$

whose solution is $a = b = 0.25p$, $\mu = -0.125$.

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NORMAL EQUATIONS

The Lagrange auxiliary function in this case is:

$$L = 2\sum_{j=1}^{k} \lambda_j \gamma(\mathbf{s}_j, \mathbf{s}_0) - \sum_{i=1}^{k}\sum_{j=1}^{k} \lambda_i \lambda_j \gamma(\mathbf{s}_i, \mathbf{s}_j) + 2\mu\left(\sum_{j=1}^{k} \lambda_j - 1\right).$$

The derivatives with respect to the unknowns are:

$$\frac{\partial L}{\partial \lambda_j} = 2\gamma(\mathbf{s}_j - \mathbf{s}_0) - \sum_{i=1}^{k} \lambda_i \gamma(\mathbf{s}_i - \mathbf{s}_j) + 2\mu = 0, \text{ for } j = 1, \ldots, k.$$

Thus

$$\boxed{\left.\begin{array}{c} \displaystyle\sum_{i=1}^{k} \lambda_i \gamma(\mathbf{s}_1, \mathbf{s}_i) - \mu = \gamma(\mathbf{s}_1, \mathbf{s}_0) \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \displaystyle\sum_{i=1}^{k} \lambda_i \gamma(\mathbf{s}_k, \mathbf{s}_i) - \mu = \gamma(\mathbf{s}_k, \mathbf{s}_0) \\ \displaystyle\sum_{i=1}^{k} \lambda_i = 1 \end{array}\right\}}$$

E. OPTIMAL ESTIMATION VARIANCE

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

$$\sum_{i=1}^{k} \lambda_i \sum_{j=1}^{k} \lambda_j \gamma(\mathbf{s}_i, \mathbf{s}_j) = \sum_{i=1}^{k} \lambda_i \gamma(\mathbf{s}_i, \mathbf{s}_0) + \mu \sum_{i=1}^{k} \lambda_i \; .$$

Because the weights sum up to 1, introducing λ_i under the second summation and replacing the resulting double summation in the general expression for the estimation variance, one obtains:

$$\sigma_{OK}^2(\mathbf{s}_0) = 2\sum_{i=1}^{k} \lambda_i \gamma(\mathbf{s}_i, \mathbf{s}_0) - \sum_{i=1}^{k} \lambda_i \gamma(\mathbf{s}_i, \mathbf{s}_0) - \mu$$

or

$$\boxed{\sigma_{OK}^2(\mathbf{s}_0) = \sum_{i=1}^{k} \lambda_i \gamma(\mathbf{s}_i, \mathbf{s}_0) - \mu \, .}$$

SUMMARY

Ordinary kriging normal equations for optimal weights λ_i :

$$\left.\begin{array}{c}\sum_{i=1}^{k}\lambda_i\gamma(\mathbf{s}_1,\mathbf{s}_i)-\mu=\gamma(\mathbf{s}_0,\mathbf{s}_1)\\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\ \sum_{i=1}^{k}\lambda_i\gamma(\mathbf{s}_k,\mathbf{s}_i)-\mu=\gamma(\mathbf{s}_0,\mathbf{s}_k)\\ \sum_{i=1}^{k}\lambda_i=1\end{array}\right\}$$

Ordinary kriging estimate:

$$z^*_{OK}(\mathbf{s}_0)=\sum_{i=1}^{n}\lambda_i z(\mathbf{s}_i)$$

Ordinary kriging mean-square-error variance:

$$\sigma^2_{OK}(\mathbf{s}_0)=\sum_{i=1}^{k}\lambda_i\gamma(\mathbf{s}_i,\mathbf{s}_0)-\mu$$

INTRINSIC MATRIX FORMULATION

$$\begin{bmatrix} \gamma(\mathbf{s}_1,\mathbf{s}_1) & \cdots & \gamma(\mathbf{s}_k,\mathbf{s}_1) & 1 \\ \vdots & \cdots & \vdots & 1 \\ \gamma(\mathbf{s}_1,\mathbf{s}_k) & \cdots & \gamma(\mathbf{s}_k,\mathbf{s}_k) & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_k \\ -\mu \end{bmatrix} = \begin{bmatrix} \gamma(\mathbf{s}_0,\mathbf{s}_1) \\ \vdots \\ \gamma(\mathbf{s}_0,\mathbf{s}_K) \\ 1 \end{bmatrix}$$

$$Z_{OK}^{*}(\mathbf{s}_0) = \begin{bmatrix} Z(\mathbf{s}_1) \\ \vdots \\ Z(\mathbf{s}_k) \\ 0 \end{bmatrix}^T \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_k \\ -\mu \end{bmatrix}$$

$$\sigma_{OK}^{2}(s_0) = \begin{bmatrix} \gamma(\mathbf{s}_0,\mathbf{s}_1) \\ \vdots \\ \gamma(\mathbf{s}_0,\mathbf{s}_k) \\ 1 \end{bmatrix}^T \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_k \\ -\mu \end{bmatrix}$$