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Estimation of Linear Combinations and Co-Kriging[1]

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Utilizing the matrix formulation of co-kriging developed previously by the author, the relationship between direct kriging of linear combinations and linear combinations of co-kriged variables is developed. Conditions for equality of the estimators and the kriging variances are examined. By presenting the problem in the context of Hilbert spaces the general relationship is clarified.

KEY WORDS: linear combinations, co-kriging, matrices, transpose, trace, kriging variance, Hilbert space, projection, inner product.

INTRODUCTION

The author (1982) has previously given the general form of co-kriging in matrix form and has given a simple method for constructing cross-covariances and cross covariograms. In addition to the possible need to separately estimate several variables, there are many instances where a linear combination may be the variable of principal interest (e.g., the sum over several geological horizons in the case of petroleum or a value function for ore, i.e., the sum of values for several metals). It is well known that kriging the linear combination directly is not optimal; Matheron (1979) has proposed the use of a correction factor and given conditions for the direct estimation of the linear combination to be optimal. In this paper the general problem is considered with application to particular models.

THE PROBLEM

Let $Z_1(x), \ldots, Z_m(x)$ be intrinsic random functions of order zero and $W(x)$ be given by

$$W(x) = \sum_{i=1}^{m} a_i Z_i(x) = \bar{Z}(x)\, A \tag{1}$$

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where

$$\bar{Z}(x) = [Z_1(x), \ldots, Z_m(x)]$$
$$A^T = [a_1, \ldots, a_m]$$

There are two ways to linearly estimate $W(x)$

(i) krige $W(x)$ directly, that is

$$W^*(x) = \sum_{j=1}^{n} \lambda_j W(x_j) \tag{2}$$

(ii) co-krige $\bar{Z}(x)$, that is co-krige $Z_1(x), \ldots, Z_m(x)$ then form

$$\hat{W}(x) = \bar{Z}^*(x)A = \sum_{j=1}^{m} Z_j^*(x)\, a_j$$

$$= \sum_{k=1}^{n} \sum_{i=1}^{m} \sum_{j=1}^{m} \lambda_{ij}^k Z_i(x_k)\, a_j \tag{3}$$

In general $W^*(x) \neq \bar{Z}^*A$ and

$$\text{Var}\ [W^*(x) - W(x)] > \text{Var}\ [\bar{Z}^*\text{A} - W(x)]$$

It is perhaps not completely obvious why this is so.

THE COKRIGING FORMULATION

Recalling the notation of Myers (1982)

$$2\gamma_{ij}(h) = \text{Cov}\ [Z_i(x+h) - Z_i(x), Z_j(x+h) - Z_j(x)]$$

$$\bar{\gamma}(h) = \begin{bmatrix} \gamma_{11}(h) \cdots \gamma_{1m}(h) \\ \gamma_{m1}(h) \cdots \gamma_{mm}(h) \end{bmatrix}$$

and we require that

$$E[\bar{Z}(x+y+h) - \bar{Z}(y)]^T[\bar{Z}(x+y) - \bar{Z}(y)]$$
$$= E[\bar{Z}(x+y) - \bar{Z}(y)]^T[\bar{Z}(x+y+h) - \bar{Z}(y)]$$

This condition is necessary because of the symmetry of $\gamma_{ij}(h)$ whereas cross-covariances may not be symmetric. The estimator for $\bar{Z}(x)$ is given by

$$\bar{Z}^*(x) = \sum_{j=1}^{n} \bar{Z}(x_j)\,\Gamma_j = [Z_1^*(x), \ldots, Z_m^*(x)], \qquad \text{where}$$

$$\sum \Gamma_j = I \tag{4}$$

and $\Sigma_{i=1}^m$ Var $[Z_i(x) - Z_i^*(x)]$ is to be minimized.

DIRECT ESTIMATION

Although it is straightforward to obtain sample variograms and subsequently fit a model directly for $W(x)$, to compare $W^*(x)$ and $\bar{Z}^*A$ we must be able to relate the coefficients, that is the systems of equations. It is useful then to first relate the variogram for $W(x)$ to the matrix variogram for $\bar{Z}(x)$. Since $W(x) = \bar{Z}(x)A$, we have

$$\begin{aligned}\gamma_W(h) &= \tfrac{1}{2} E[W(x+h) - W(x)]^2 \\ &= \tfrac{1}{2} E[\bar{Z}(x+h)A - \bar{Z}(x)A]^T[\bar{Z}(x+h)A - \bar{Z}(x)A] \\ &= A^T\{\tfrac{1}{2} E[\bar{Z}(x+h) - \bar{Z}(x)]^T[\bar{Z}(x+h) - \bar{Z}(x)]\}A \\ &= A^T\bar{\gamma}(h)A \end{aligned} \tag{5}$$

A similar result for covariances is obtained if the Z_is are second-order stationary. Note that the kriging variance for W^* is given by

$$\sigma^2_{K,D} = \sum A^T\bar{\gamma}(x - x_j)A\,\lambda_j + \mu \tag{6}$$

where

$$\sum_{j=1}^{n} A^T\bar{\gamma}_{ij}A\,\lambda_j + \mu = A^T\bar{\gamma}_jA$$

$$\sum_{j=1}^{n} \lambda_j = 1 \tag{7}$$

ESTIMATION BY CO-KRIGING

If $\bar{Z}(x)$ is estimated by $\bar{Z}^*(x)$, then $W(x)$ is estimated by

$$\hat{W}(x) = \bar{Z}^*\mathrm{A} = \sum Z(x_j)\,\Gamma_jA$$

and the variance of the error, that is

$$\mathrm{Var}\,[\hat{W}(x) - W(x)]$$

is given by

$$\sigma^2_{K,J} = \sum A^T\bar{\gamma}_{ij}\Gamma_jA + A^T\bar{\mu}A \tag{8}$$

where

$$\sum_{j=1}^{n} \bar{\gamma}_{ij}\Gamma_j + \bar{\mu} = \bar{\gamma}_i$$

$$\sum_{j=1}^{n} \Gamma_j = I \tag{9}$$

Note that $\sigma^2_{K,J}$ is not quite a kriging variance, that is, the Γ_js were obtained by minimizing

$$E[\bar{Z}(x) - \bar{Z}^*(x)]\ [\bar{Z}(x) - \bar{Z}^*(x)]^T$$

and not by minimizing

$$E[\bar{Z}(x) - \bar{Z}^*(x)]\ AA^T\ [\bar{Z}(x) - \bar{Z}^*(x)]^T$$
$$= E[A^T[\bar{Z}(x) - \bar{Z}^*(x)]^T[\bar{Z}(x) - \bar{Z}^*(x)]\ A]$$

RELATIONSHIP OF THE KRIGING SYSTEMS

By considering (7) against (9), (6) against (8), and (1) against (2) we see that $A\ \lambda_j = \Gamma_j A$ for all j is a sufficient condition for the kriging system to be equivalent, for $W(x) = W^*(x)$ and $\sigma^2_{K,D} = \sigma^2_{K,J}$. Since A is not square, and hence not invertible, the condition is dependent on A.

ANOTHER PERSPECTIVE

From the point of view of better understanding why $W \neq W^*$ in general it may be easier to place the problem in the context of projection in a Hilbert space. Let $H_1, \ldots, H_m$ be copies of a real $L^2(\Omega, \ \ , P)$ where P is a probability measure and the inner product in L^2 is $E[XY] = \langle X, Y\rangle$, $\bar{Z}(x)$ may be viewed as an element of the exterior sum $\bar{H} = H_1 + H_2 + \cdots + H_m$. If $\langle\ ,\ \rangle_i$ is the inner product in H_i, the inner product $\bar{H}$ is the sum $\Sigma\langle\ ,\ \cdot\rangle_i$, that is

$$\langle \bar{Z}(x), \bar{Z}(y)\rangle = \sum_{i=1}^{m} \langle Z_i(x), Z_i(y)\rangle_i \tag{10}$$

Let L_i be the closed linear subspace of H_i generated by authorized linear combinations of the elements $Z_j(x_k)$; $j = 1, \ldots, m$; $k = 1, \ldots, n$. The joint estimation of $Z_1(x), \ldots, Z_m(x)$, that is, of $\bar{Z}(x)$, is the projection of $\bar{Z}(x)$, as an element of $\bar{H}$, onto the subspace $\bar{L} = L_1 + \cdots + L_m$, using the inner product of $\bar{H}$.

To contrast joint estimation with separate variable estimation let L_i^o be the linear subspace of H_i generated by the authorized linear combinations of the elements $Z_i(x_k)$; $k = 1, \ldots, n$. Clearly $L_i^o \subset L^i$ and hence $\bar{L}^o = L_1^o + \cdots + L_m^o \subset \bar{L}$.

If we let $\Pi_{\bar{L}}$, $\Pi_{\bar{L}^o}$ denote the projection operators onto the subspaces $\bar{L}$, $\bar{L}^o$, respectively, then clearly

$$\|\bar{Z}(x) - \Pi_{\bar{L}}\bar{Z}(x)\|^2 \leqslant \|\bar{Z}(x) - \Pi_{\bar{L}^o}\bar{Z}(x)\|^2 \tag{11}$$

We can also describe the relationship between $\bar{Z}^*(x)\ A$ and $W^*(x)$ as estimators of $\bar{Z}(x)\ A$ in the context of Hilbert spaces. The matrix A determines a linear mapping of $\bar{H}$ into H, H a copy of L^2. Likewise $\mathfrak{A}$ maps $\bar{L}$ into L, a linear space of H. However, in general

$$\mathfrak{A}\ \Pi_{\bar{L}} \neq \Pi_L \mathfrak{A} \tag{12}$$

We can present this pictorially as follows

$$\begin{array}{ccc} \bar{H} & \xrightarrow{\mathfrak{A}} & H \\ \downarrow & & \downarrow \\ \bar{L} & \xrightarrow{\mathfrak{A}} & L \end{array}$$

and the relationship between $\mathfrak{A}\Pi_{\bar{L}}$, $\Pi_L \cdot \mathfrak{A}$ is expressed by noting that (13) is not a commutative diagram.

$\mathfrak{A}\Pi_{\bar{L}}$ represents first forming linear combinations and then kriging the linear combination. $\Pi_{\bar{L}}\, \mathfrak{A}$ represents co-kriging, then forming the linear combination.

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