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Cross Validation of Kriging in a Unique Neighborhood[1]

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Cross validation is an appropriate tool for testing interpolation methods: it consists of leaving out one data point at a time, and determining how well this point can be estimated from the other data. Cross validation is often used for testing "moving neighborhood" kriging models; in this case, each unknown value is predicted from a small number of surrounding data. In "unique neighborhood" kriging algorithms, each estimation uses all the available data; as a result, cross validation would spend much computer time. For instance, with n *data points it would cost at least the resolution of* n *systems of* n × n *linear equations (each with a different matrix). Here, we present a much faster method for cross validation in a unique neighborhood. Instead of solving* n *systems* n × n, *it only requires the inversion of one* n × n *matrix. We also generalized this method to leaving out several points instead of one.*

KEY WORDS: cross validation, kriging, moving neighborhood, unique neighborhood.

INTRODUCTION

To perform a kriging, one often has the choice between different structural models. For instance, in nonstationary geostatistics, one can use a fit of the variogram of the residuals, or a generalized covariance (which may have been computed by the geostatistical package BLUEPACK).

To test each model, a good method is to use "cross validation": each at a time, the values at data points x_α are kriged, as if they were unknown. Then, one can compare the true values $z(x_\alpha)$ with their estimates $z^*(x_\alpha)$, and decide (for instance) to keep the model which gives the lowest mean squared error

$$\frac{1}{n} \sum_{\alpha=1}^{n} [z(x_\alpha) - z^*(x_\alpha)]^2$$

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In addition to the estimate, kriging gives a standard deviation $\sigma(x_\alpha)$ of the error at point x_α. One can test if the sum

$$\frac{1}{n} \sum_{\alpha=1}^{n} \left[\frac{z(x_\alpha) - z^*(x_\alpha)}{\sigma(x_\alpha)}\right]^2$$

which measures the quality of the error prevision, is close to 1 or not.

In a moving neighborhood, each kriged point is estimated by a linear combination of the values at its nearest neighbors. Generally, one uses about the 15 nearest neighbors. So, for instance in two dimensions with a parabolic drift, each kriging requires the resolution of a $(15 + 6) \times (15 + 6)$ system of linear equations (there are six non-bias conditions).

In a unique neighborhood, each point is estimated by a linear combination of all the other data. For instance, in two dimensions with a parabolic drift and $n = 100$ data, each estimation requires the resolution of a 106×106 system. Cross validation of a model would require the resolution of 100 systems 106×106 (with a different matrix each time), which would be very expensive. That is why cross validation is used in a unique neighborhood only for small sets of data. However, cross validation would be very helpful, first, because it is impossible to make a good statistical inference of global structural models (cross validation would be an objective way of testing them) and second, because maps obtained by kriging in a unique neighborhood are much more "smooth" and aesthetic than those obtained in a moving neighborhood. So, by cross validating moving and unique neighborhood krigings for a given structural model, we could test if the gain in smoothness implies a gain, or loss, in accuracy.

THE KRIGING SYSTEM

Consider a variable $z(x)$ which is a realization of a random function $Z(x)$ such that

$$\begin{cases} E[Z(x)] = m(x) \\ \text{Var } [Z(x+h) - Z(x)] = 2\gamma(h) \end{cases}$$

If x is a point on a plane, we call u and v its coordinates: $x = (u, v)$; in three dimensions $x = (u, v, w)$. If the drift $m(x)$ is a polynomial of degree k in the coordinates of x, we can write

$$m(x) = \sum_{l=0}^{m} a_l f^l(x)$$

where the $f^l(x)$ are monomials of degree lower or equal to k. For example, if we work on a plane with a parabolic drift

$$m(x) = m(u, v) = a_0 + a_1 u + a_2 v + a_3 u^2 + a_4 uv + a_5 v^2$$

we have

$$m = 5 \qquad f^0(x) = 1$$
$$f^1(x) = u \qquad f^2(x) = v$$
$$f^3(x) = u^2 \qquad f^4(x) = uv \qquad f^5(x) = v^2$$

With universal kriging we estimate the value at a point x by a linear combination of the values at n data points

$$Z^*(x) = \sum_{\alpha=1}^{n} \lambda^\alpha Z(x_\alpha)$$

The λ^α must be such that

$$\begin{cases} E[Z^*(x)] = E[Z(x)] & \text{(non-bias condition)} \\ \text{Var } [Z(x) - Z^*(x)] \text{ minimum} & \text{(optimality condition)} \end{cases}$$

And the system which gives them is (Matheron 1971)

$$\begin{cases} \sum_{\alpha=1}^{n} \lambda^\alpha \gamma(x_\alpha - x_\beta) + \sum_{l=0}^{m} \mu_l f^l(x_\beta) = \gamma(x_\beta - x) & (\forall \beta \in (1, \ldots, n)) \\ \sum_{\alpha=1}^{n} \lambda^\alpha f^l(x_\alpha) = f^l(x) & (\forall l \in (0, \ldots, m)) \end{cases} \quad (1)$$

- The μ_l are some Lagrange multipliers which are also unknown.
- If $m = 0$, we find the well-known ordinary kriging system (Journel and Huijbregts, 1978). If we were working with a generalized covariance $K(h)$ instead of a variogram, we would just have to replace γ by K everywhere in the system (Delfiner and Delhomme, 1973). So this system is general; it includes the stationary case and the generalized covariance case. All the results deduced from this system will also be general.
- In the following, we will often use some simplified notations

$$\gamma_{\alpha\beta} = \gamma(x_\alpha - x_\beta), \qquad f_\beta^l = f^l(x_\beta), \qquad z_\alpha = z(x_\alpha)$$

KRIGING AS AN INTERPOLATOR

In a unique neighborhood, the left-hand side of the system (1) does not depend on the kriged point x: only the right-hand side does. Hence, kriging in a unique neighborhood can also be interpreted as a function of the kriged point x (Matheron, 1971; Dubrule, 1981).

$$z^*(x) = \sum_{\alpha=1}^{n} b^\alpha \gamma(x - x_\alpha) + \sum_{l=0}^{m} c_l f^l(x)$$

The coefficients b^α and c_l being determined by the system

$$\begin{cases} \sum_{\alpha=1}^{n} b^\alpha \gamma(x_\alpha - x_\beta) + \sum_{l=0}^{m} c_l f^l(x_\beta) = z(x_\beta), & (\forall \beta \in (1, \ldots, n)) \\ \sum_{\alpha=1}^{n} b^\alpha f^l(x_\alpha) = 0 & (\forall l \in (0, \ldots, m)) \end{cases} \quad (2)$$

(The first set of conditions simply means that kriging must honor data points.)

Using matrices, system (2) can be written

$$\begin{bmatrix} \gamma_{11} & \gamma_{12} \cdots \gamma_{1n} & f_1^o \cdots f_1^m \\ \gamma_{21} & \gamma_{22} \cdots \gamma_{2n} & f_2^o \cdots f_2^m \\ \vdots & \vdots \quad \vdots & \vdots \quad \vdots \\ \gamma_{n1} & \gamma_{n2} \cdots \gamma_{nn} & f_n^o \cdots f_n^m \\ f_1^o & f_2^o \cdots f_n^o & \\ \vdots & \vdots \quad \vdots & \bigcirc \\ f_1^m & f_2^m \cdots f_n^m & \end{bmatrix} \begin{bmatrix} b^1 \\ b^2 \\ \vdots \\ b^n \\ c_o \\ \vdots \\ c_m \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (3)$$

If we suppose that the value at datum point x_{α_o} is unknown, the new interpolating function will be

$$z^{*\prime}(x) = \sum_{\alpha \neq \alpha_o} b'^\alpha \gamma(x - x_\alpha) + \sum_{l=0}^{m} c'_l f^l(x)$$

with

$$\begin{cases} \sum_{\alpha \neq \alpha_o} b'^\alpha \gamma(x_\alpha - x_\beta) + \sum_{l=0}^{m} c'_l f^l(x_\beta) = z(x_\beta) & [\forall \beta \in (1, \ldots, n), \beta \neq \alpha_o] \\ \sum_{\alpha \neq \alpha_o} b'^\alpha f^l(x_\alpha) = 0 & [\forall l \in (0, \ldots, m)] \end{cases}$$

This can be written

$$\begin{bmatrix} \gamma_{11} \cdots \gamma_{1,\alpha_o-1} & \gamma_{1,\alpha_o+1} \cdots \gamma_{1n} & f_1^o & \cdots f_1^m \\ \vdots & \vdots & \vdots & \vdots \\ \gamma_{\alpha_o-1,1} \cdots & \cdots \gamma_{\alpha_o-1,n} & f_{\alpha_o-1}^o & \cdots f_{\alpha_o-1}^m \\ \gamma_{\alpha_o+1,1} \cdots & \cdots \gamma_{\alpha_o+1,n} & f_{\alpha_o+1}^o & \cdots f_{\alpha_o+1}^m \\ \vdots & \vdots & \vdots & \vdots \\ \gamma_{n1} \cdots \gamma_{n,\alpha_o-1} & \gamma_{n,\alpha_o+1} \cdots \gamma_{nn} & f_n^o & \cdots f_n^m \\ f_1^o \cdots f_{\alpha_o-1}^o & f_{\alpha_o+1}^o \cdots f_n^o & & \\ \vdots & \vdots & \bigcirc & \\ f_1^m \cdots f_{\alpha_o-1}^m & f_{\alpha_o+1}^m \cdots f_n^m & & \end{bmatrix} \times \begin{bmatrix} b'^1 \\ \vdots \\ b'^{\alpha_o-1} \\ b'^{\alpha_o+1} \\ \vdots \\ b'^n \\ c'_o \\ \vdots \\ c'_m \end{bmatrix} = \begin{bmatrix} z_1 \\ \vdots \\ z_{\alpha_o-1} \\ z_{\alpha_o+1} \\ \vdots \\ z_n \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{4}$$

SOLUTION OF THE PROBLEM

The $(n+m) \times (n+m)$ matrix (4) is obtained by deleting line and column α_o of the $(n+m+1) \times (n+m+1)$ matrix (3). The question is: instead of separately solving all the systems (4), for each $\alpha_o \in \{1, \ldots, n\}$, would it be possible to invert matrix (3) once for all, and, from its inverse, deduce the solutions of systems (4)? In fact, we do not need to really invert systems (4): we only want to be able to compute $z^{*\prime}(x_{\alpha_o})$, for each α_o

$$z^{*\prime}(x_{\alpha_o}) = \sum_{\alpha \neq \alpha_o} b'^{\alpha} \gamma(x_\alpha - x_{\alpha_o}) + \sum_{l=0}^{m} c'_l f^l(x_{\alpha_o})$$

System (4) can be written

$$\begin{bmatrix}
\gamma_{11} & \cdots \gamma_{1,\alpha_o-1} & \gamma_{1,\alpha_o} & \gamma_{1,\alpha_o+1} & \cdots \gamma_{1n} & f_1^o & \cdots f_1^m \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\gamma_{\alpha_o-1,1} & & & & \gamma_{\alpha_o-1,n} & f_{\alpha_o-1}^o & \cdots f_{\alpha_o-1}^m \\
\gamma_{\alpha_o,1} & \vdots & \vdots & \vdots & \gamma_{\alpha_o,n} & f_{\alpha_o}^o & \cdots f_{\alpha_o}^m \\
\gamma_{\alpha_o+1,1} & & & & \gamma_{\alpha_o+1,n} & f_{\alpha_o+1}^o & \cdots f_{\alpha_o+1}^m \\
\vdots & & & & \vdots & \vdots & \vdots \\
\gamma_{n,1} & \cdots \gamma_{n,\alpha_o-1} & \gamma_{n,\alpha_o} & \gamma_{n,\alpha_o+1} & \cdots \gamma_{nn} & f_n^o & \cdots f_n^m \\
f_1^o & \cdots f_{\alpha_o-1}^o & f_{\alpha_o}^o & f_{\alpha_o+1}^o & \cdots f_n^o & & \\
\vdots & \vdots & \vdots & \vdots & \vdots & & \bigcirc \\
f_1^m & \cdots f_{\alpha_o-1}^m & f_{\alpha_o}^m & f_{\alpha_o+1}^m & \cdots f_n^m & &
\end{bmatrix}$$

$$\times \begin{bmatrix} b'^1 \\ \vdots \\ b'^{\alpha_o-1} \\ 0 \\ b'^{\alpha_o+1} \\ \vdots \\ b'^n \\ c_1' \\ \vdots \\ c_m' \end{bmatrix} = \begin{bmatrix} z_1 \\ \vdots \\ z_{\alpha_o-1} \\ z^{*\prime}(x_{\alpha_o}) \\ z_{\alpha_o+1} \\ \vdots \\ z_n \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{5}$$

Matrix (3) is symmetric. So is its inverse, which we can write in a block configuration

$$\begin{bmatrix}
b^{11} & b^{12} \cdots b^{1n} & \lambda_o^1 & \cdots \lambda_m^1 \\
b^{21} & b^{22} \cdots b^{2n} & \lambda_o^2 & \cdots \lambda_m^2 \\
\vdots & \vdots \quad \vdots & \vdots & \vdots \\
b^{n1} & b^{n2} \cdots b^{nn} & \lambda_o^n & \cdots \lambda_m^n \\
\lambda_o^1 & \lambda_o^2 \cdots \lambda_o^n & \mu_{oo} & \cdots \mu_{om} \\
\lambda_1^1 & \lambda_1^2 \cdots \lambda_1^n & \mu_{1o} & \cdots \mu_{1m} \\
\vdots & \vdots \quad \vdots & \vdots & \vdots \\
\lambda_m^1 & \lambda_m^2 \cdots \lambda_m^n & \mu_{mo} & \cdots \mu_{mm}
\end{bmatrix} \tag{6}$$

And we get, after the α_o^{th} line of system (5):

$$0 = \sum_{\alpha \neq \alpha_o} b^{\alpha_o \alpha} z_\alpha + b^{\alpha_o \alpha_o} z^{*\prime}(x_{\alpha_o})$$

And

$$z^{*\prime}(x_{\alpha_o}) = - \sum_{\alpha \neq \alpha_o} \frac{b^{\alpha_o \alpha}}{b^{\alpha_o \alpha_o}} z(x_\alpha) \tag{7}$$

This is the result we were expecting: using the inverse of matrix (3), it is possible to compute $z^{*\prime}(x_{\alpha_o})$, for each $\alpha_o \in \{1, \ldots, n\}$. So, instead of solving system (4) for each point x_{α_o} (with a different matrix at each time), one has only to calculate the inverse of matrix (3). And this inverse can be reused later: for, if the variogram model corresponding to matrix (3) is finally selected for kriging, matrix (3) will be the matrix of the kriging system. Formula (7) also shows that the kriging weights for the estimation of $z(x_{\alpha_o})$ on the basis of the $z(x_\alpha)$ $(\alpha \neq \alpha_o)$ are respectively

$$\lambda^\alpha = - \frac{b^{\alpha_o \alpha}}{b^{\alpha_o \alpha_o}}$$

We can also compute the kriging variance

$$\begin{aligned}
&\operatorname{Var}\,[Z(x_{\alpha_o}) - Z^{*\prime}(x_{\alpha_o})] \\
&= \operatorname{Var}\left[Z(x_{\alpha_o}) + \sum_{\alpha \neq \alpha_o} \frac{b^{\alpha_o \alpha}}{b^{\alpha_o \alpha_o}} Z(x_\alpha)\right] \\
&= \operatorname{Var}\left[\sum_{\alpha=1}^{n} \frac{b^{\alpha_o \alpha}}{b^{\alpha_o \alpha_o}} Z(x_\alpha)\right] \\
&= - \sum_{\alpha=1}^{n} \sum_{\beta=1}^{n} \frac{b^{\alpha_o \alpha} b^{\alpha_o \beta}}{b^{\alpha_o \alpha_o^2}} \gamma(x_\alpha - x_\beta)
\end{aligned}$$

(if we worked with a covariance or generalized covariance $K(h)$, we would have to replace $-\gamma$ by K)

$$= - \sum_{\alpha=1}^{n} \frac{b^{\alpha_o \alpha}}{b^{\alpha_o \alpha_o^2}} \sum_{\beta=1}^{n} b^{\alpha_o \beta} \gamma(x_\alpha - x_\beta)$$

But matrix (6) is the inverse of matrix (3). So, we have

$$\sum_{\beta=1}^{n} b^{\alpha_o \beta} \gamma(x_\alpha - x_\beta) = \delta_\alpha^{\alpha_o} - \sum_{l=o}^{m} \lambda_l^{\alpha_o} f_\alpha^l$$

($\delta_\alpha^{\alpha_o}$ is equal to 1 if $\alpha_o = \alpha$, 0 if $\alpha_o \neq \alpha$):

And

$$-\sum_{\alpha=1}^{n} \frac{b^{\alpha_o\alpha}}{b^{\alpha_o\alpha_o^2}} \sum_{\beta=1}^{n} b^{\alpha_o\beta}\, \gamma(x_\alpha - x_\beta) = -\frac{1}{b^{\alpha_o\alpha_o}} + \sum_{l=0}^{m} \frac{\lambda_l^{\alpha_o}}{b^{\alpha_o\alpha_o^2}} \sum_{\alpha=1}^{n} b^{\alpha_o\alpha} f_\alpha^l$$

But, because (6) is the inverse of (3), we have

$$\sum_{\alpha=1}^{n} b^{\alpha_o\alpha} f_\alpha^l = 0$$

And we get

$$\text{Var}\,[Z(x_{\alpha_o}) - Z^{*\prime}(x_{\alpha_o})] = -\frac{1}{b^{\alpha_o\alpha_o}}$$

If we worked with a covariance, or generalized covariance, instead of a variogram, we would find

$$\text{Var}\,[Z(x_{\alpha_o}) - Z^{*\prime}(x_{\alpha_o})] = +\frac{1}{b^{\alpha_o\alpha_o}} \tag{8}$$

CASES OF SINGULARITY

Until now, we supposed that

$$b^{\alpha_o\alpha_o} \neq 0 \qquad (\forall\, \alpha_o \in \{1 - - n\})$$

Is it possible to find an α_o such that

$$b^{\alpha_o\alpha_o} = 0?$$

We know that $b^{\alpha_o\alpha_o}$ is a diagonal term of the inverse of matrix (3). So

$$b^{\alpha_o\alpha_o} = \frac{\det\,(A_{\alpha_o\alpha_o})}{\det A}$$

where A is the matrix (3), and $A_{\alpha_o\alpha_o}$ is the matrix obtained by deleting line and column α_o of matrix (3), $A_{\alpha_o\alpha_o}$ is exactly the matrix (4). So, we have the equivalence $b^{\alpha_o\alpha_o} = 0 \Longleftrightarrow \det\,(A_{\alpha_o\alpha_o}) = 0 \Longleftrightarrow$ system (4) has no solution so

$$b^{\alpha_o\alpha_o} = 0 \Longleftrightarrow z^{*\prime}(x_{\alpha_o}) \text{ is undetermined}$$

This result is quite logical; as soon as $z^{*\prime}(x_{\alpha_o})$ exists, it can be calculated using formula (7).

GENERALIZING THE CROSS VALIDATION TO MORE THAN ONE POINT

Let us suppose now that two data points x_{α_o} and x_{α_1} are unknown. On the basis of the $(n-2)$ other data $z(x_\alpha)$ $(\alpha \in \{1 - - n\}, \alpha \neq \alpha_o, \alpha_1)$ kriging at a point x can be written

$$z^{*''}(x) = \sum_{\substack{\alpha \neq \alpha_o \\ \alpha \neq \alpha_1}} b''^{\alpha} \gamma(x - x_\alpha) + \sum_{l=0}^{m} c''_l f^l(x)$$

with

$$\begin{cases} \displaystyle\sum_{\substack{\alpha \neq \alpha_o \\ \alpha \neq \alpha_1}} b''^{\alpha} \gamma_{\alpha\beta} + \sum_{l=0}^{m} c''_l f^l_\beta = z_\beta & (\forall \beta \in \{1 - - n\}, \beta \neq \alpha_o, \alpha_1) \\ \displaystyle\sum_{\substack{\alpha \neq \alpha_o \\ \alpha \neq \alpha_1}} b''^{\alpha} f^l_\alpha = 0 & (\forall l \in \{0 - - m\}) \end{cases}$$

This can be written the same way as (5)

$$\begin{bmatrix} \gamma_{11} & \cdots \gamma_{1,\alpha_o} & \cdots \gamma_{1,\alpha_1} & \cdots \gamma_{1n} & f^o_1 & \cdots f^m_1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \gamma_{\alpha_o,1} & \cdots \gamma_{\alpha_o,\alpha_o} & \cdots \gamma_{\alpha_o,\alpha_1} & \cdots \gamma_{\alpha_o,n} & f^o_{\alpha_o} & \cdots f^m_{\alpha_o} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \gamma_{\alpha_1,1} & \cdots \gamma_{\alpha_1,\alpha_o} & \cdots \gamma_{\alpha_1,\alpha_1} & \cdots \gamma_{\alpha_1,n} & f^o_{\alpha_1} & \cdots f^m_{\alpha_1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \gamma_{n,1} & \cdots \gamma_{n,\alpha_o} & \cdots \gamma_{n,\alpha_1} & \cdots \gamma_{n,n} & f^o_n & \cdots f^m_n \\ f^o_1 & \cdots f^o_{\alpha_o} & \cdots f^o_{\alpha_1} & \cdots f^o_n & & \\ \vdots & \vdots & \vdots & \vdots & \multicolumn{2}{c}{\bigcirc} \\ f^m_1 & \cdots f^m_{\alpha_o} & \cdots f^m_{\alpha_1} & \cdots f^m_n & & \end{bmatrix} \begin{bmatrix} b''^1 \\ \vdots \\ 0 \\ \vdots \\ 0 \\ \vdots \\ b''^n \\ c''_o \\ \vdots \\ c''_m \end{bmatrix} = \begin{bmatrix} z_1 \\ \vdots \\ z^{*''}(x_{\alpha_o}) \\ \vdots \\ z^{*''}(x_{\alpha_1}) \\ \vdots \\ z_n \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

After the (α_o)th and (α_l)th lines we get

$$\begin{cases} b^{\alpha_o\alpha_o} z^{*''}(x_{\alpha_o}) + b^{\alpha_o\alpha_1} z^{*''}(x_{\alpha_1}) = - \displaystyle\sum_{\substack{\alpha \neq \alpha_o \\ \alpha \neq \alpha_1}} b^{\alpha_o\alpha} z(x_\alpha) \\ b^{\alpha_1\alpha_o} z^{*''}(x_{\alpha_o}) + b^{\alpha_1\alpha_1} z^{*''}(x_{\alpha_1}) = - \displaystyle\sum_{\substack{\alpha \neq \alpha_o \\ \alpha \neq \alpha_1}} b^{\alpha_1\alpha} z(x_\alpha) \end{cases} \tag{9}$$

If

$$\begin{vmatrix} b^{\alpha_o\alpha_o} & b^{\alpha_o\alpha_1} \\ b^{\alpha_1\alpha_o} & b^{\alpha_1\alpha_1} \end{vmatrix} \neq 0$$

The values of $z^{*''}(x_{\alpha_o})$ and $z^{*''}(x_{\alpha_1})$ are obtained by solving the (2×2) system (9).

It can be proved (see appendix) that, as for the one-point case, the determinant of (9) is null only if $z^{*''}(x_{\alpha_o})$ and $z^{*''}(x_{\alpha_1})$ are undetermined.

This result can be generalized to more than two points: if we suppose that the p data points $x_{\alpha_o}, x_{\alpha_1} -- x_{\alpha_{p-1}}$ are unknown, the kriging estimates $z^{*(p)}(x_{\alpha_o}), --- z^{*(p)}(x_{\alpha_{p-1}})$ can be calculated by inverting the $(p \times p)$ system

$$\sum_{j=0}^{p-1} b^{\alpha_i\alpha_j} z^{*(p)}(x_{\alpha_j}) = - \sum_{\alpha \neq \alpha_o -- \alpha_{p-1}} b^{\alpha_i\alpha} z(x_\alpha), \qquad (\forall\, i \in \{o -- (p-1)\}) \tag{10}$$

The determinant of this system is

$$\begin{vmatrix} b^{\alpha_o\alpha_o} & \cdots\, b^{\alpha_o\alpha_{p-1}} \\ \vdots & \vdots \\ b^{\alpha_{p-1}\alpha_o} & \cdots\, b^{\alpha_{p-1}\alpha_{p-1}} \end{vmatrix}$$

It is equal to zero only if the kriging system without the p points $x_{\alpha_o} -- x_{\alpha_{p-1}}$ has no solution (see appendix).

APPENDIX

We prove here that the determinant of system (10) is null only if the kriging matrix based on the $(n - p)$ points $(x_\alpha, \alpha \neq \alpha_o, \alpha_1, --, \alpha_{p-1})$ is singular. To obtain this result, we prove the following proposition.

Consider a $(n + m + 1) \times (n + m + 1)$ matrix A, that we write in a block configuration

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

where

A_{11} is a $p \times p$ matrix
A_{12} is a $p \times (n + m + 1 - p)$ matrix

A_{21} is a $(n + m + 1 - p) \times p$ matrix
A_{22} is a $(n + m + 1 - p) \times (n + m + 1 - p)$ matrix

We make the hypothesis that both matrices A_{22} and A are nonsingular. We are going to prove that, if

$$B = A^{-1} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

we have the identity

$$\det B_{11} = \frac{\det A_{22}}{\det A}$$

This result will be a generalization of the case $p = 1$, where it is a well-known result that, if b^{22} is a diagonal term of A^{-1}, we have

$$b^{22} = \frac{\det A_{22}}{\det A}$$

Proof. A can be written

$$A = \begin{pmatrix} C_{11} & X \\ 0 & I_{n+m+1-p} \end{pmatrix} \times \begin{pmatrix} I_p & 0 \\ Y & A_{22} \end{pmatrix}$$

(I_p and $I_{m+n+1-p}$ are the $p \times p$ and $(m + n + 1 - p) \times (m + n + 1 - p)$ identity matrices).

To obtain such a decomposition, we simply have to take

$$\begin{array}{lll} A_{11} = C_{11} + XY & X = A_{12}A_{22}^{-1} & (A_{22} \text{ is nonsingular}) \\ A_{12} = XA_{22} \quad \Rightarrow & Y = A_{21} & \\ A_{21} = Y & C_{11} = A_{11} - A_{12}A_{22}^{-1}A_{21} & \end{array}$$

So, we have

$$\det A = \det C_{11} \det A_{22} \tag{A1}$$

But

$$B = A^{-1} = \begin{pmatrix} I_p & 0 \\ Y & A_{22} \end{pmatrix}^{-1} \times \begin{pmatrix} C_{11} & X \\ 0 & I_{n+m+1-p} \end{pmatrix}^{-1}$$

From equality (A_1), C_{11} is nonsingular, and we can also write

$$B = A^{-1} = \begin{pmatrix} I_p & 0 \\ Z & A_{22}^{-1} \end{pmatrix} \times \begin{pmatrix} C_{11}^{-1} & T \\ 0 & I_{m+n+1-p} \end{pmatrix}$$

(The exact expression of the Z and T matrices does not matter) so

$$B_{11} = C_{11}^{-1}$$

$$\Rightarrow \det B_{11} = 1/\det C_{11}$$

And, after (A_1), we get

$$\det B_{11} = \frac{\det A_{22}}{\det A}$$

Take for A the matrix of the global kriging system, using the n data (matrix 3), and make the decomposition

$$A = \left[\begin{array}{ccc|ccc|cc}
\gamma_{11} & \cdots & \gamma_{1p} & \gamma_{1,p+1} & \cdots & \gamma_{1n} & f_1^o & \cdots f_1^m \\
\vdots & & \vdots & \vdots & & \vdots & \vdots & \vdots \\
\gamma_{p1} & \cdots & \gamma_{pp} & \gamma_{p,p+1} & \cdots & \gamma_{pn} & f_p^o & \cdots f_p^m \\
\hline
\gamma_{p+1,1} & \cdots & \gamma_{p+1,p} & \gamma_{p+1,p+1} & \cdots & \gamma_{p+1,n} & f_{p+1}^o & \cdots f_{p+1}^m \\
\vdots & & \vdots & \vdots & & \vdots & \vdots & \vdots \\
\gamma_{n,1} & \cdots & \gamma_{n,p} & \gamma_{n,p+1} & \cdots & \gamma_{n,n} & f_n^o & \cdots f_n^m \\
f_1^o & \cdots & f_p^o & f_{p+1}^o & \cdots & f_n^o & & \\
\vdots & & \vdots & \vdots & & \vdots & & \bigcirc \\
f_1^m & \cdots & f_p^m & f_{p+1}^m & \cdots & f_n^m & &
\end{array}\right]$$

In this case A_{22} is the kriging matrix corresponding the $n - p$ data x_{p+1} -- x_n (of course, we do not lose generality by supposing that the p data which are supposed unknown are the p first ones).

From matrix (6), we see that

$$B_{11} = \begin{pmatrix} b^{11} & \cdots & b^{1p} \\ \vdots & & \vdots \\ b^{p1} & \cdots & b^{pp} \end{pmatrix}$$

So

$$\left.\begin{array}{l}\text{Matrix } A_{22} \text{ nonsingular} \\ \det A_{22} \neq 0\end{array}\right\} \Rightarrow \det B_{11} = \frac{\det A_{22}}{\det A} \neq 0 \Rightarrow \text{system (10) nonsingular}$$

And the system (10) is nonsingular as soon as the kriging system without the p points is nonsingular.

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