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How to rewrite multivariate random functions as univariate to do cokriging. The theory

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Abstract

In 2005 Martínez-Vargas formulated a pure heterotopic cokriging to estimate a regionalized random function (RF) $Z^*(x)$, defined as a linear combination of n univariate RFs $Z_i(x)$, which coefficients $\mathbf{1}_i(x)$ are indicator variables of a disjoint set of categories i. An apparent contradiction appear in this model, because it assumes that cross covariances exists in the same location despite its heterotopic nature. To evade any confusion or contradiction the multivariate set of RF $Z_i(x)$ was rewritten as $Z(x,i)$, been the points (x,i) and (x,j) non-coincident when i and j are unequal. The heterotopy was considered as an omission of $Z(x,.)$ in the data and in the target, non-imposed by the model. The result is then a particular case of the classical cokriging method. With this notation the classical cokriging system was rewritten as the kriging system of the univariate RF $Z(x,i)$, assuming that attached to this RF exists a drif $m(x,i,j)$. The members $f_l(x,i,j)$ of $m(x,i,j)$ can be linearly independents or dependents. Through this notation the multivariate formulation of kriging is reduced to an univariate system, the existence of more than one variable or the presence of heterotopy does not introduce extra handling to build the equations of the kriging system, increasing the computational efficiency.

Key words

Cokriging, geostatistics, heterotopy, multivariate system, regionalized random function.

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Como reescribir funciones aleatorias multivariadas como univariadas para hacer cokrigeage. La teoría

Resumen

En el año 2005 Martínez-Vargas formuló un sistema de cokrigeage puro heterotópico para estimar una función aleatoria regionalizada (RF) $Z^*(x)$ definida como la combinación lineal de n RF's univariadas $Z_i(x)$, cuyos coeficientes $\mathbf{1}_i(x)$ son indicatrices de un set disyuntivo de categorías i. Aparentemente este modelo se contradice pues asume que las covarianzas cruzadas existen en un mismo punto, a pesar de su carácter puramente heterotópico. Para evadir dicha contradicción se redefinió el set de RF $Z_i(x)$ como una única RF $Z(x,i)$, siendo los puntos (x,i) y (x,j) no coincidentes si i y j no son iguales. La heterotopía fue simplemente considerada como una omisión de la RF $Z(x,.)$ en los datos y en los puntos a estimar, no impuesta por el modelo; entonces el resultado es simplemente un caso particular del cokrigeage clásico. Con esta notación se reescribió el sistema de cokrigeage clásico como el sistema de krigeage de la RF univariada $Z(x,i)$, asumiendo que esta posee un *drift* definido como $m(x,i,j)$, donde los miembros $f_l(x,i,j)$ de $m(x,i,j)$ pueden ser linealmente dependientes o independientes. Bajo esta notación el sistema de krigeage se reduce a un sistema univariado, la existencia de más de una variable o la presencia de heterotropía no impone la necesidad de manipulaciones extras para definir el sistema de ecuaciones de krigeage, incrementándose la eficiencia computacional.

Palabras clave

Cokrigeage, función aleatoria regionalizada, geoestadística, heterotopía, sistema multivariado.

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INTRODUCTION

In 2005, Martínez-Vargas, with the aim to reduce the effect of the mixture of statistical populations of iron grades in a lateritic deposit, during the estimation with cokriging, rewrote the global iron grades as a linear combination defined as:

$$Fe(v) = p_1 Fe_1(v) + p_2 Fe_2(v) + p_3 Fe_3(v), \quad (1)$$

$$Fe(x_0) = \mathbf{1}_1 Fe_1(x_0) + \mathbf{1}_2 Fe_2(x_0) + \mathbf{1}_3 Fe_3(x_0), \quad (2)$$

where Fe is the iron global grade, v and x_0 are the block and punctual support; Fe_1, Fe_2, Fe_3 are the iron grades associated to the three lithologies existing in the deposit; p_1, p_2, p_3 are the proportions of those lithologies in v and $\mathbf{1}_1$, $\mathbf{1}_2$, $\mathbf{1}_3$ are the indicator variables for the punctual support.

The data in this model is purely heterotopic, due to the fact that the categories 1, 2 and 3 are disjoint. For this reason Martínez-Vargas (2005) developed a procedure to fit the cross members of the pure heterotopic variogram. Because in the model with block support the kriging estimator depends on the proportions p_i, Martínez-Vargas (2005) replaced the block model by a punctual discretization, $Fe(v)$ was obtained as a mean $E[Fe(x_i)], \forall x_i \in v$, of the elements $Fe(x_i)$ calculated as the equation (2). In 2006 Martínez-Vargas showed that this approach reduces the error not only globally but per lithology. In addition he defined the model as:

> Given a random function $Z(x)$, for example iron grades, the proportions $p_i(x)$ of lithologies i in the point with coordinates vector x and the indicator function $\mathbf{1}_i(x)$ defined for the categories i; to separate the mixture of statistical populations in punctual support the RF $Z(x)$ can be written as:

$$Z(x)=\sum_{i=1}^{n} p_i(x)Z_i(x)=\sum_{i=1}^{n}\mathbf{1}_i(x)Z_i(x)=Z_{i_0}(x), \tag{3}$$

assuming $p_i(x)\ \forall i$ is known for any point x the estimator is:

$$Z^*(x)=\sum_{i=1}^{n} p_i(x)Z_i^*(x)=\sum_{i=1}^{n}\mathbf{1}_i(x)Z_i^*(x)=Z_{i_0}^*(x), \tag{4}$$

where:

$$\mathbf{1}_i(x)=\begin{cases}1 & \text{if } i=i_0\\ 0 & \text{otherwise}\end{cases}$$

$Z_{i_0}^*(x)$ is the estimator of the RF corresponding to the lithology i_0, existing in the point x.

With those assumptions $Z^*(x)$ does not depends on proportions $p_i(x)$, neither on the indicators $\mathbf{1}_i(x)$.

Martínez-Vargas (2006) also showed that in punctual support the cokriging can be implemented as a classic pure heterotopic cokriging; this is not the case for block support.

The estimator defined in the equation (3) requires that the covariance $\mathrm{Cov}(Z_i(x_\alpha);Z_j(x_\beta))\ \forall\ i,j,x_\beta,x_\alpha\in v$ exists, but at the first view this is contradictory because the coexistence in a point of $Z_i(x);Z_j(x)\ \forall\ i\neq j$ is negated by the equation (3). Then our questions are: -is this model wrong?-, -it is possible to redefine or rewrite the multivariate set of RF in a non contradictory way with its own definition?-, -if it is possible, what are the implications to the definition of the cokriging system?-.

METHODOLOGY

Chilès & Delfiner (1999, p. 12) gave a definition of regionalized random function as:

Given a domain $D\subset R^n$, with a positive volume, and a probability space (Ω,A,P), a random function (abbreviation:

RF) is a function of two variables $Z(x,\omega)$ such that for each $x \in D$ the section $Z(x,\circ)$ is a random variable on (Ω,A,P). Each of the functions $Z(\circ,\omega)$ defined on D as the section of the RF at $\omega \in \Omega$ is a realization of the RF.

In the multivariate case we have a set of RF $Z_i(x)$, defined in the same domain $D \subset R^n$, with positive volume, and multivariate probability space (Ω_m, A_m, P_m). The fundamental idea to solve the contradiction of coexistence of $Z_i(x); Z_j(x) \quad \forall \quad i \neq j$, for the model proposed in the equation (3) is to consider the RFs $Z_i(x)$ as a single RF $Z(x,i)$, therefore the punctual pure heterotopic system can be rewritten as shows the equation 5:

$$Z(x) = Z(x, i_0), \qquad (5)$$

because $Z(x,i) \; \forall \, i \neq i_0$ does not exist, and this is a condition not imposed by the model but by data. Similarly the selection of a specific target $Z(x_0, i_0)$ is not lying in the definition of the model, but in the choice of the target.

The idea of a RF $Z(x,i)$ was also proposed by Chilès & Delfiner (1999, p. 297), to extend the RF definition given by Matheron (1970), with the objective to show that the cokriging error is orthogonal to the kriging estimator.

Under this assumption $(x,i) \neq (x,j) \quad \forall \, i \neq j$, they are not-coincident, therefore the variance of any linear combination of the random functions $Z(x,i), Z(x,j) \quad \forall \, i \neq j$ is (semi)definite positive. The pure heterotopy must be regarded as a special case on data, and the coexistence of $Z(x,i), Z(x,j)$ is not contradictory any more. This is a necessary condition to extend the model to the block support, but this is out of the scope of this paper.

To define the cokriging system of intrinsic random functions of order *k* (IRF-*k)*, we consider three possibilities of four possible types of drift (as state Chilès & Delfiner 1999, p. 298): (a) algebraically independents drifts, (b) algebraically dependents drifts, and (c) the mix case of (a) and (b); in case (d) are the drifts non linearly related, but these can not be handled by the linearity of the cokriging system.

The drift of the RF $Z(x,i)$ for the point (x,i), if exist, may be written as:

$$m(x,i,\mathrm{j})=\sum_{l=0} a_l f_l(x,i,j_l)=\sum_{l=0} a_l \mathbf{1}(i,j_l) f_l(x,i),$$

where $\mathrm{j}=[j_{0,},...,j_l,...,j_t]$ is the vector of variable identifiers associated to each one of the t monomials, $f_l(j_l)$ is a deterministic function known at any point (x,i). This notation is valid for all stationary forms of RFs, including the special cases of the external drift and the non existence of drift $m(x,i,\mathrm{j})=\varnothing \quad \forall x,i,j_l$, that conduces to simple cokriging.

The random variables $z(x,\omega_{0,}i)$, are the random variables z_i, in x, where ω_0 is the realization measured or known (Chilès and Delfiner, 1999, p. 12). To write the kriging system of $Z(x,i)$, we proceed to join the sets $z_i(x,\omega_0)$, as it shows Figure 1.

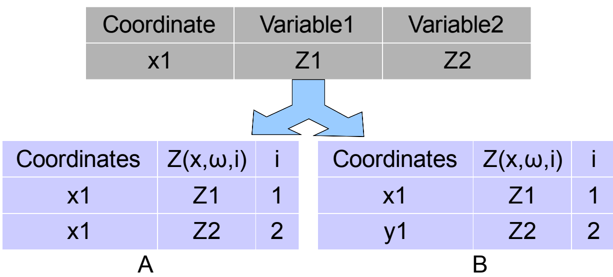

Figure 1. Transformation of a multivariate set $\mathrm{Variable1}(x,\omega_0)$, $\mathrm{Variable2}(x,\omega_0)$ in one univariate $z(x,\omega_{0,}i)$, where x is the coordinate vector in a Hilbert space, i relates the RF $Z(x,i)$ with $Z_i(x)$, A and B are equivalent definitions, both show that $(x_{1,}\omega_0,1)\neq(x_{1,}\omega_0,2)$

The equation (6) is the resulting general estimator of the univariate RF $Z(x,i)$, with drift $m(x,i,\mathrm{j})$. The total number of drifts in the case of all monomials linearly independent is $t=(k+1)n_i$, where k is the order of the drift (zero for the ordinary kriging and -1 for simple kriging), n_i is the number of categories i. The system of equations (7) minimizes the estimation variance of the error $err=Z^*(x_{0,}i_0)-Z(x_{0,}i_0)$, where $K^{i,j}_{(x,i)(x,j)}$ is the variogram, covariance or generalized covariance between $Z(x,i)$ and $Z(x,j)$.

$$Z^*(x_0,i_0)=\sum_{i,x}\lambda^i_x Z(x,i) \tag{6}$$

$$\begin{bmatrix} K^{i,j}_{(x,i)(x,j)} & f(x,j,\mathrm{i}) \\ f(x,i,\mathrm{j}) & 0 \end{bmatrix}\begin{bmatrix} \lambda^j_{(x,i)} \\ \mu^l_i \end{bmatrix}=\begin{bmatrix} K^{i_0,j}_{(x_0,i_0),(x,j)} \\ f(x_0,i_0,\mathrm{j}) \end{bmatrix} \tag{7}$$

DISCUSSION

A consequence of this notation is that the cokriging multivariate system of the RF $Z_i(x)$ is reduced to the univariate kriging of the RF $Z(x,i)$. This simplifies the algorithm of construction of the system of kriging equations. Those implications are shown through an example defined in Figure 2.

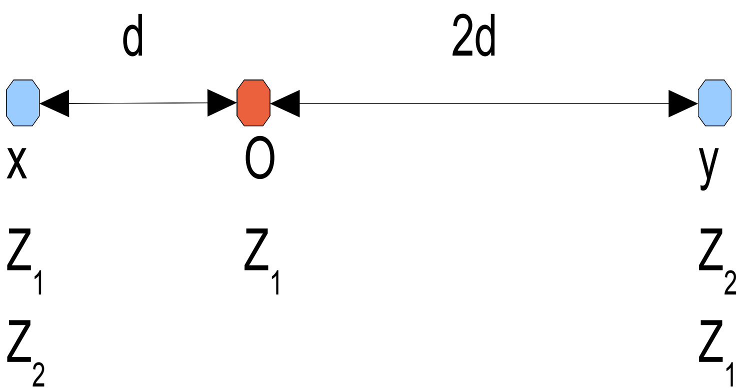

Figure 2. Schematic representation of the data and the target point.

To simplify the notation the coordinates are written as sub-indexes, and the variable identifiers as super-indexes. For example $C^{12}_{x_1y_1}$ is the covariance between variables v_1 and v_2 in the points x_1, and y_2, or better, between $Z(x_{1,}1)$ and $Z(x_{2,}2)$; if we write coordinates as super-index, for example $C^{x_1y_1}_{x_1y_1}$, is to highlight that the lithology i comes from the point defined by the tuple (x,i), from now written as x_i in many cases.

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The simple cokriging of the RF Z1(x) and Z2(x)

In this example the data is defined as a classical bivariate set, as shows in Table 1 and Figure 2.

Table 1. Data used to define the cokriging system, NaN means *'Not a Number'*.

Coordinate	**Variable1**	**Variable2**
Data		
x	Z1	Z2
y	Z1	Z2
Target		
O	Z1	NaN

In matrix notation the cokriging system is a defined as:

$$\begin{bmatrix} C_{xx}^{11} & C_{xy}^{11} & \vdots & C_{xx}^{12} & C_{xy}^{12} \\ C_{yx}^{11} & C_{yy}^{11} & \vdots & C_{yx}^{12} & C_{yy}^{12} \\ \cdots & \cdots & & \cdots & \cdots \\ C_{xx}^{21} & C_{yx}^{21} & \vdots & C_{xx}^{22} & C_{xy}^{22} \\ C_{yx}^{21} & C_{yy}^{21} & \vdots & C_{yx}^{22} & C_{yy}^{22} \end{bmatrix} \begin{bmatrix} \lambda_x^1 \\ \lambda_y^1 \\ \cdots \\ \lambda_x^2 \\ \lambda_y^2 \end{bmatrix} = \begin{bmatrix} C_{Ox}^{11} \\ C_{Oy}^{11} \\ \cdots \\ C_{Ox}^{12} \\ C_{Oy}^{12} \end{bmatrix}$$

This system can be constructed by the classical cokriging definition, as the union of four matrices $C_{x_a x_b}^{ij}$, but when we have more than 3-4 variables and partial heterotopy it is necessary to eliminate columns and rows, with an extra computational cost; for example if $z_2(x) = \mathrm{NaN}$, the system is as follow:

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$$\begin{bmatrix} C_{xx}^{11} & C_{xy}^{11} & \vdots & C_{xy}^{12} \\ C_{yx}^{11} & C_{yy}^{11} & \vdots & C_{yy}^{12} \\ \cdots & \cdots & & \cdots \\ C_{yx}^{21} & C_{yy}^{21} & \vdots & C_{yy}^{22} \end{bmatrix} \begin{bmatrix} \lambda_x^1 \\ \lambda_y^1 \\ \cdots \\ \lambda_y^2 \end{bmatrix} = \begin{bmatrix} C_{Ox}^{11} \\ C_{Oy}^{11} \\ \cdots \\ C_{Oy}^{12} \end{bmatrix}$$

Two extra steeps are necessary:1) delete one row and one col, and 2) rearrange the elements of the matrix.

The simple kriging system for the RF Z(*x, i*)

The data defined with notation $Z(x,i)$ is as shows Table 2.

Table 2. Data in Table 1, rewritten as notation $Z(x,i)$.

Tuple (x, i)	**Variable**	**Mapping index (mi)**
Data		
x,1	Z1	1
y,1	Z1	2
x,2	Z2	3
y,2	Z2	4
Target		
O, 1	Z1	0

The simple kriging defined with the data in Table 2, is simpler than the cokriging defined with the data in Table 1. Each element of the covariance matrix $C_{x_i y_j}^{ij}$ is directly mapped through the mapping index *mi* and its associated tuple (x,i). We proceed similarly with the kriging coefficients ($\lambda_{x_i}^{i}$) and the covariance vector ($C_{Ox_i}^{ij}$), being the system defined as:

$$\begin{bmatrix} C^{11}_{x_1x_1} & C^{11}_{x_1y_1} & \vdots & C^{12}_{x_1x_2} & C^{12}_{x_1y_2} \\ C^{11}_{y_1x_1} & C^{11}_{y_1y_1} & \vdots & C^{12}_{y_1x_2} & C^{12}_{y_1y_2} \\ \cdots & \cdots & & \cdots & \cdots \\ C^{21}_{x_2x_1} & C^{21}_{x_2y_1} & \vdots & C^{22}_{x_2x_2} & C^{22}_{x_2y_2} \\ C^{21}_{y_2x_1} & C^{21}_{y_2y_1} & \vdots & C^{22}_{y_2x_2} & C^{22}_{y_2y_2} \end{bmatrix} \begin{bmatrix} \lambda^1_{x_1} \\ \lambda^1_{y_1} \\ \cdots \\ \lambda^2_{x_2} \\ \lambda^2_{y_2} \end{bmatrix} = \begin{bmatrix} C^{11}_{Ox_1} \\ C^{11}_{Oy_1} \\ \cdots \\ C^{12}_{Ox_2} \\ C^{12}_{Oy_2} \end{bmatrix}$$

If the system is partially heterotopic, it is automatically defined through the mapping index mi. For example if $z(x,2) = \mathrm{NaN}$, the data is defined as shows Table 3. The kriging system with data shown in Table 3 is:

$$\begin{bmatrix} C^{11}_{x_1x_1} & C^{11}_{x_1y_1} & \vdots & C^{12}_{x_1y_2} \\ C^{11}_{y_1x_1} & C^{11}_{y_1y_1} & \vdots & C^{12}_{y_1y_2} \\ \cdots & \cdots & & \cdots \\ C^{21}_{y_2x_1} & C^{21}_{y_2y_1} & \vdots & C^{22}_{y_2y_2} \end{bmatrix} \begin{bmatrix} \lambda^1_{x_1} \\ \lambda^1_{y_1} \\ \cdots \\ \lambda^2_{y_2} \end{bmatrix} = \begin{bmatrix} C^{11}_{Ox_1} \\ C^{11}_{Oy_1} \\ \cdots \\ C^{12}_{Oy_2} \end{bmatrix}$$

Table 3. Data on Table 2, redefined for $z(x,2) = \mathrm{NaN}$.

Tuple (x, i)	**Variable**	**Mapping index (mi)**
Data		
x,1	Z1	1
y,1	Z1	2
y,2	Z2	3
Target		
O, 1	Z1	0

Notice that if we change the order of mi the system is equivalent, does not change the result.

The ordinary kriging system of the RF Z(*x*, *i*)

For the ordinary kriging system of the RF $Z(x,i)$, we assume a drift of type (a) as $m(x,i,\mathrm{j}) = a_0 \mathbf{1}(i, j_l)$, to satisfy the condition $\sum_{x_i} \lambda_x^i = \mathbf{1}(i_0, j)$. The data on Table 2, is then redefined as it shows Table 4. To simplify the notation we write $\mathbf{1}(x,i,j_l) = \mathbf{1}_{\mathbf{j}}^{xi}$, which is equal to one when $i = j_l$ and equal to zero otherwise.

The kriging with linear independents drifts of order zero is defined as follow:

$$
\begin{bmatrix}
C_{x_1x_1}^{11} & C_{x_1y_1}^{11} & \vdots & C_{x_1x_2}^{12} & C_{x_1y_2}^{12} & \vdots & \mathbf{1}_1^{x_1} & \mathbf{1}_2^{x_1} \\
C_{y_1x_1}^{11} & C_{y_1y_1}^{11} & \vdots & C_{y_1x_2}^{12} & C_{y_1y_2}^{12} & \vdots & \mathbf{1}_1^{y_1} & \mathbf{1}_2^{y_1} \\
\cdots & \cdots & & \cdots & \cdots & & \cdots & \cdots \\
C_{x_2x_1}^{21} & C_{x_2y_1}^{21} & \vdots & C_{x_2x_2}^{22} & C_{x_2y_2}^{22} & \vdots & \mathbf{1}_1^{x_2} & \mathbf{1}_2^{x_2} \\
C_{y_2x_1}^{21} & C_{y_2y_1}^{21} & \vdots & C_{y_2x_2}^{22} & C_{y_2y_2}^{22} & \vdots & \mathbf{1}_1^{y_2} & \mathbf{1}_2^{y_2} \\
\cdots & \cdots & & \cdots & \cdots & & \cdots & \cdots \\
\mathbf{1}_1^{x_1} & \mathbf{1}_1^{y_1} & \vdots & \mathbf{1}_1^{x_2} & \mathbf{1}_1^{y_2} & \vdots & 0 & 0 \\
\mathbf{1}_2^{x_1} & \mathbf{1}_2^{y_1} & \vdots & \mathbf{1}_2^{x_2} & \mathbf{1}_2^{y_2} & \vdots & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\lambda_{x_1}^1 \\ \lambda_{y_1}^1 \\ \cdots \\ \lambda_{x_2}^2 \\ \lambda_{y_2}^2 \\ \cdots \\ \mu_{\mathbf{1}_1}^1 \\ \mu_{\mathbf{1}_2}^2
\end{bmatrix}
=
\begin{bmatrix}
C_{Ox_1}^{11} \\ C_{Oy_1}^{11} \\ \cdots \\ C_{Ox_2}^{12} \\ C_{Oy_2}^{12} \\ \cdots \\ \mathbf{1}_1^{O_1} \\ \mathbf{1}_2^{O_1}
\end{bmatrix}
$$

Notice that the construction process is then similar to this used for simple kriging, the mapping index mi extend the drifts idea as two extra data samples, but with a different function, in this case $\mathbf{1}(x,i,j_l)$, instead $C_{x_i y_j}^{ij}$.

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Table 4. Redefinition of the data of Table 2, to cover the ordinary kriging conditions.

Tuple (x, i)	**Variable**	**Mapping index (mi)**
Data		
x,1	Z1	1
y,1	Z1	2
x,2	Z2	3
y,2	Z2	4
Drift		
$\mathbf{1}(x,i,j_l)$, $i=1$	$\mathbf{1}_1^{xj}$	5
$\mathbf{1}(x,i,j_l)$, $i=2$	$\mathbf{1}_2^{xj}$	6
Target		
O, 1	Z1	0_1
$\mathbf{1}(x,i,j)$, $i=1$	$\mathbf{1}_1^{xj}$	0_2

The IRF-k (k>1) and the universal kriging systems of RF Z(*x, i*)

To handle drifts of order k greater than one, we have to define a set of $n_i(k+1)$ monomials multiplied by $\mathbf{1}(x,i,j_l)$, for the case of linear independent member of the drifts, plus the n_d linear dependent members of the drifts. The procedure is then similar to the one applied to the ordinary kriging of the RF $Z(x,i)$. This includes the case the external drift monomials.

Finally, to do cokriging with extended collocation we have to include in the data section of the Table a row for $Z(x_{0,}c)$, where x_0 is the target coordinate and $c \neq i_0$ is the index of the collocated variable.

CONCLUSIONS

To avoid any contradiction between the model presented by Martínez-Vargas (2005, 2006) and the assumption that all cross covariances exist at any point x, the pure heterotopic nature of the data and the target must be regarded as a condition imposed by the data and not by the model. This assumption is enhanced by the univariate notation of multivariate RFs defined as $Z(x,i)$.

To rewrite a multivariate set of RFs $Z_i(x)$ as a single univariate RF $Z(x,i)$ with a drift $m(x,i,\mathrm{j})$ simplifies the construction of the system of kriging equations and increases the computational efficiency. The resulting system of equations is equivalent to the system obtained by the classical multivariate approach.

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