Xavier Emery

Multigaussian kriging for point-support estimation: incorporating constraints on the sum of the kriging weights

Abstract In the geostatistical analysis of regionalized data, the practitioner may not be interested in mapping the unsampled values of the variable that has been monitored, but in assessing the risk that these values exceed or fall short of a regulatory threshold. This kind of concern is part of the more general problem of estimating a transfer function of the variable under study. In this paper, we focus on the multigaussian model, for which the regionalized variable can be represented (up to a nonlinear transformation) by a Gaussian random field. Two cases are analyzed, depending on whether the mean of this Gaussian field is considered known or not, which lead to the simple and ordinary multigaussian kriging estimators respectively. Although both of these estimators are theoretically unbiased, the latter may be preferred to the former for practical applications since it is robust to a misspecification of the mean value over the domain of interest and also to local fluctuations around this mean value. An advantage of multigaussian kriging over other nonlinear geostatistical methods such as indicator and disjunctive kriging is that it makes use of the multivariate distribution of the available data and does not produce order relation violations. The use of expansions into Hermite polynomials provides three additional results: first, an expression of the multigaussian kriging estimators in terms of series that can be calculated without numerical integration; second, an expression of the associated estimation variances; third, the derivation of a disjunctive-type estimator that minimizes the variance of the error when the mean is unknown.

Keywords Gaussian random fields · Multivariate normality · Conditional expectation · Ordinary kriging · Lognormal kriging · Hermite polynomials

X. Emery (✉)
Department of Mining Engineering, University of Chile,
Avenida Tupper 2069, Santiago, Chile
E-mail: xemery@cec.uchile.cl
Tel.: +56-2-9784498
Fax: +56-2-6723504

Introduction

In many fields of application concerned with spatial prediction, the practitioner needs to determine the distribution of values of a regionalized variable relative to one or several thresholds. For instance, in soil and groundwater remediation studies, the environmentalist looks whether the concentration of a pollutant exceeds a critical level (specified by regulators) or not. In agricultural land management, the soil scientist is interested in avoiding a deficiency in nutrients or an excess in contaminant concentrations. In mineral resource and ore reserve evaluation, the mining engineer wants to assess the grades of the elements of interest, by-products and impurities relative to given economic or regulatory cut-offs.

Although it is helpful to map the regionalized variable, linear kriging is generally not suitable for all these applications concerned with the risk of exceeding or falling short of a threshold (Chilès and Delfiner 1999, p. 178). Instead, nonlinear geostatistical methods can be used, such as indicator, disjunctive and multigaussian kriging (Matheron 1976; Journel 1983; Verly 1983, 1984; Maréchal 1984). However, disjunctive and multigaussian kriging are still not widely used in practical applications. One of the reasons is that they are traditionally restricted to simple kriging, i.e. kriging with a known mean, which is often considered a demanding requirement (Guibal and Remacre 1984, p. 434; Rivoirard 1994, p. 67).

The objective of this work is to develop and improve the multigaussian approach, in particular concerning the possibility to use ordinary kriging (i.e. kriging with an unknown mean) instead of simple kriging. After a brief recall of the definition and main properties of the multigaussian model, the multigaussian kriging approach is introduced, distinguishing the cases of a known and an unknown mean. Then we examine the precision of the estimators and calculate the associated error variances. Further developments are finally proposed to construct

an "optimal" estimator that minimizes the error variance when the mean is unknown.

Principles and properties of multigaussian kriging

The multigaussian model

The regionalized variable under study is regarded as a realization of a (nonlinear) transform of a random field $\{Y_{\mathbf{x}}, \mathbf{x} \in R^d\}$ with univariate Gaussian distribution (Rivoirard 1994, p. 46; Goovaerts 1997, p. 273). Usually, one works with standard Gaussian variables, i.e. the mean and variance of $Y_{\mathbf{x}}$ are set to 0 and 1, respectively. As this paper examines the case of an unknown mean, here we prefer to assume that the mean is equal to m, whereas the variance of $Y_{\mathbf{x}}$ is still one.

The key assumption of the multigaussian model is that the random field $\{Y_{\mathbf{x}}, \mathbf{x} \in R^d\}$ has a multivariate Gaussian spatial distribution. Such distribution is fully determined as soon as the mean value and the correlogram (or variogram) are identified, which makes the model very simple to use for nonlinear estimation as well as for stochastic simulation. Given a set of data transformed to normal scores values, a key question is to check the plausibility of the multigaussian assumption. A possibility is to use one of the many tests for multivariate normality proposed in the statistical literature (e.g. Koziol 1986; Mecklin and Mundfrom 2004), although such tests are not widely used in geostatistical applications. Alternatively, the multigaussian hypothesis can be validated by examining the experimental bivariate distributions of the normal scores values, for which several tools are available:

1. Inspection of the lagged-scattergrams for several lag separation vectors and calculation of regression curves associated with the Hermite polynomials of low degrees (Rivoirard 1994, p. 39; Chica-Olmo and Luque-Espinar 2002).
2. Inspection of the indicator variograms associated with several thresholds (Goovaerts 1997, p. 278).
3. Inspection of the variograms of several orders, e.g. by comparing the madogram and the rodogram to the classical variogram (Emery 2005a). These tools are interesting when the mean value is assumed unknown, since they do not work with the random field $\{Y_{\mathbf{x}}, \mathbf{x} \in R^d\}$ itself, but with its increments. The objective of multigaussian kriging is to estimate a function of the regionalized variable at an unsampled location $\mathbf{x}$, which is also a function of the normal score transform $Y_{\mathbf{x}}$, denoted by $\varphi(Y_{\mathbf{x}})$ henceforth; this function is sometimes called a "transfer function" or a "recovery function". For instance, the problem mentioned in the introductory section (assessment of whether the value of the variable under study exceeds a critical threshold or not) is dealt with by considering an indicator function:

$$\varphi(Y_{\mathbf{x}}) = \begin{vmatrix} 1 & \text{if } Y_{\mathbf{x}} \geqslant y \\ 0 & \text{otherwise.} \end{vmatrix} \tag{1}$$

The correlogram $\rho(\mathbf{x},\mathbf{x}')$ of the Gaussian field $\{Y_{\mathbf{x}}, \mathbf{x} \in R^d\}$ is supposed to be correctly modeled and the available information to perform the local estimation are the values of this field at a set of sampling locations, say $\{\mathbf{x}_\alpha, \alpha = 1,..., n\}$. In the following, two cases are distinguished, depending on whether the mean value m is considered known or not.

Case of a known mean

In the case of a known mean, the posterior distribution of $Y_{\mathbf{x}}$ at location $\mathbf{x}$, i.e. its distribution conditioned to the data located at $\{\mathbf{x}_\alpha, \alpha = 1,..., n\}$, is Gaussian-shaped with a mean equal to the simple kriging $Y_{\mathbf{x}}^{SK}$ from the normal scores data and variance equal to the corresponding simple kriging variance $(\sigma_{\mathbf{x}}^{SK})^2$ (Goovaerts 1997, p. 272; Chilès and Delfiner 1999, p. 381). One can therefore write:

$$Y_{\mathbf{x}} = Y_{\mathbf{x}}^{SK} + \sigma_{\mathbf{x}}^{SK} T, \tag{2}$$

where T is a standard Gaussian random variable independent of the data (this is the standardized simple kriging error).

Simple multigaussian kriging (in short, sMK) is defined by taking the expected value of the posterior distribution of $\varphi(Y_{\mathbf{x}})$: this estimator is also known as the "conditional expectation" of $\varphi(Y_{\mathbf{x}})$ (Rivoirard 1994, p. 61; Chilès and Delfiner 1999, p. 380). Using Eq. 2, one finds:

$$[\varphi(Y_{\mathbf{x}})]^{sMK} = \int \varphi(Y_{\mathbf{x}}^{SK} + \sigma_{\mathbf{x}}^{SK} t) \, g(t) \, dt, \tag{3}$$

where $g(.)$ is the standard Gaussian probability density function. An equivalent expression is the following one:

$$[\varphi(Y_{\mathbf{x}})]^{sMK} = E\{\varphi(Y_{\mathbf{x}}^{SK} + \sigma_{\mathbf{x}}^{SK} T)|Y_{\mathbf{x}}^{SK}\} \tag{4}$$

which shows that all the conditioning information is actually contained in the simple kriging estimator. The integral in Eq. 3 can be evaluated via numerical integration (Verly 1984, p. 500).

The simple multigaussian kriging estimator has several interesting properties:

1. It is unbiased, i.e. the expected value of the error is zero.
2. It is conditionally unbiased (Chilès and Delfiner 1999, p. 164), i.e. the expected value of $\varphi(Y_{\mathbf{x}})$ knowing its estimate is equal to this estimate:

$$E\left\{\varphi(Y_{\mathbf{x}}) \mid [\varphi(Y_{\mathbf{x}})]^{sMK}\right\} = [\varphi(Y_{\mathbf{x}})]^{sMK}. \tag{5}$$

3. It honors the values of $\varphi(Y_{\mathbf{x}})$ at the sample locations (indeed, at a data location, the kriging estimator matches the datum and the kriging variance is zero).
4. The simple kriging estimator tends to the prior mean m and the kriging variance to the prior unit variance

when the distance between $\mathbf{x}$ and the data is greater than the range of the correlogram. Hence, far from the data, the conditional expectation of $\varphi(Y_{\mathbf{x}})$ converges to its prior expectation. Note that this property is necessary to ensure conditional unbiasedness (property 2). Indeed, far from the data, the conditioning is inactive in Eq. 5, so one has:

$$\begin{aligned} [\varphi(Y_{\mathbf{x}})]^{\text{sMK}} &= E\left\{\varphi(Y_{\mathbf{x}})|[\varphi(Y_{\mathbf{x}})]^{\text{sMK}}\right\} \\ &\approx E\{\varphi(Y_{\mathbf{x}})\}. \end{aligned} \tag{6}$$

5. The estimation error $\varphi(Y_{\mathbf{x}}) - [\varphi(Y_{\mathbf{x}})]^{\text{sMK}}$ is not correlated with the estimator $[\varphi(Y_{\mathbf{x}})]^{\text{sMK}}$ (Chilès and Delfiner 1999, p. 15), which entails the following identity:

$$\text{cov}\left\{\varphi(Y_{\mathbf{x}}), [\varphi(Y_{\mathbf{x}})]^{\text{sMK}}\right\} = \text{var}\left\{[\varphi(Y_{\mathbf{x}})]^{\text{sMK}}\right\}. \tag{7}$$

Simple multigaussian kriging relies on the mean value m of the Gaussian field $\{Y_{\mathbf{x}}, \mathbf{x} \in R^d\}$, a feature that may be undesirable in practical applications (Remacre 1984; Guibal and Remacre 1984, p. 434). In the next subsection, the hypotheses on which the model is based are weakened, by considering the mean unknown.

Case of an unknown mean

This situation is of interest when the random field $\{Y_{\mathbf{x}}, \mathbf{x} \in R^d\}$ has a varying mean that can be considered constant only at the scale of the kriging neighborhood (case of local stationarity). Usually, this local mean has to be estimated from the data contained in the neighborhood and the estimation may be poor if these data are too few or highly clustered in space. Should the estimated mean differ from the true mean of $\{Y_{\mathbf{x}}, \mathbf{x} \in R^d\}$, the simple multigaussian kriging estimator would be biased, hence there is a risk of getting inaccurate estimations of the transfer functions.

Considering an unknown mean avoids this inconvenient as the model does no longer rely on this mean and accounts for the uncertainty associated with it. This approach is widely applied in linear geostatistics, where ordinary kriging is commonly used instead of simple kriging. The ordinary kriging of $Y_{\mathbf{x}}$ is defined by the following weighting of the normal scores data:

$$Y_{\mathbf{x}}^{\text{OK}} = \sum_{\alpha=1}^{n} \lambda_{\alpha}^{\text{OK}} Y_{\mathbf{x}_{\alpha}} \tag{8}$$

with

$$\begin{cases} \sum_{\beta=1}^{n} \lambda_{\beta}^{\text{OK}} \rho(\mathbf{x}_{\alpha}, \mathbf{x}_{\beta}) + \mu_{\mathbf{x}} = \rho(\mathbf{x}_{\alpha}, \mathbf{x}) \; \forall \alpha = 1 \ldots n \\ \sum_{\alpha=1}^{n} \lambda_{\beta}^{\text{OK}} = 1. \end{cases} \tag{9}$$

The ordinary kriging variance (variance of the estimation error) is

$$(\sigma_{\mathbf{x}}^{\text{OK}})^2 = 1 - \sum_{\alpha=1}^{n} \lambda_{\alpha}^{\text{OK}} \rho(\mathbf{x}_{\alpha}, \mathbf{x}) - \mu_{\mathbf{x}}. \tag{10}$$

Ordinary multigaussian kriging is defined by substituting ordinary kriging to simple kriging in Eq. 3. However, to avoid bias, the simple kriging variance has to be replaced by the ordinary kriging variance plus twice the Lagrange multiplier introduced in Eq. 9 (Emery 2005b, 2006):

$$[\varphi(Y_{\mathbf{x}})]^{\text{oMK}} = \int \varphi\left(Y_{\mathbf{x}}^{\text{OK}} + \sqrt{(\sigma_{\mathbf{x}}^{\text{OK}})^2 + 2\mu_{\mathbf{x}}} \, t\right) g(t) \, dt. \tag{11}$$

This estimator does not depend on the value of the mean any more. It can be re-written in the following form:

$$[\varphi(Y_{\mathbf{x}})]^{\text{oMK}} = E\left\{\varphi\left(Y_{\mathbf{x}}^{\text{OK}} + \sqrt{(\sigma_{\mathbf{x}}^{\text{OK}})^2 + 2\mu_{\mathbf{x}}} \, T\right)|Y_{\mathbf{x}}^{\text{OK}}\right\}, \tag{12}$$

where T stands for a standard Gaussian random variable independent of $Y_{\mathbf{x}}^{\text{OK}}$. Note that this is not the standardized ordinary kriging error, since this error is correlated to the data and therefore to the kriging estimator (Chilès and Delfiner 1999, p. 184). The unbiasedness of ordinary multigaussian kriging can be demonstrated by noting that $Y_{\mathbf{x}}^{\text{OK}}$ is a Gaussian random variable, as a weighted average of data with a multivariate Gaussian distribution, with mean m and variance (Eqs. 8, 9, 10)

$$(s_{\mathbf{x}}^{\text{OK}})^2 = \text{var}(Y_{\mathbf{x}}^{\text{OK}}) = 1 - (\sigma_{\mathbf{x}}^{\text{OK}})^2 - 2\mu_{\mathbf{x}}. \tag{13}$$
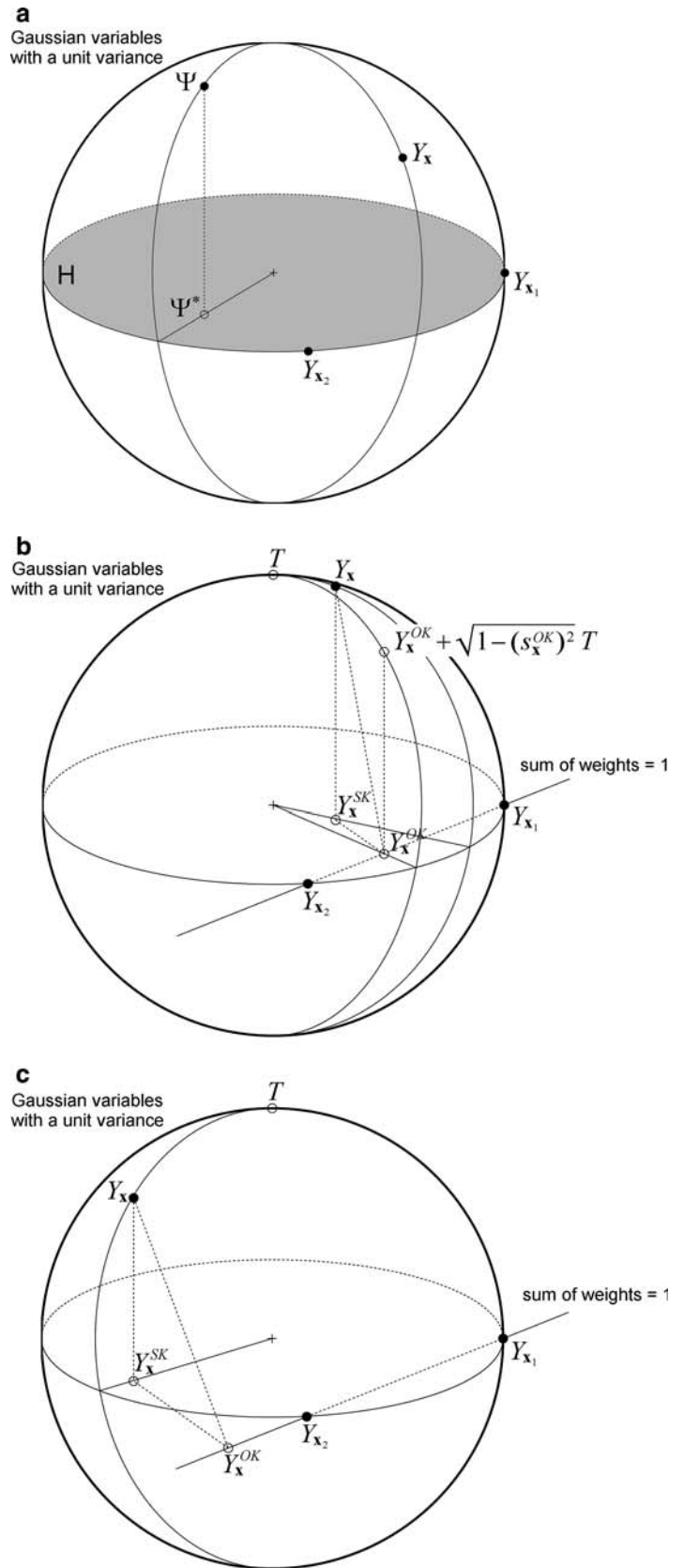
Consequently, $Y_{\mathbf{x}}^{\text{OK}} + \sqrt{(\sigma_{\mathbf{x}}^{\text{OK}})^2 + 2\mu_{\mathbf{x}}} \, T$ has the same prior distribution as $Y_{\mathbf{x}}$ (namely, a normal distribution with mean m and unit variance). Hence the expected value of the estimator in Eq. 12 is equal to the one of the function to estimate, irrespective of the value of the mean m:

$$\begin{aligned} E\left\{[\varphi(Y_{\mathbf{x}})]^{\text{oMK}}\right\} &= E\left\{\varphi\left(Y_{\mathbf{x}}^{\text{OK}} + \sqrt{(\sigma_{\mathbf{x}}^{\text{OK}})^2 + 2\mu_{\mathbf{x}}} \, T\right)\right\} \\ &= E\{\varphi(Y_{\mathbf{x}})\}. \end{aligned} \tag{14}$$

Remarks

1. Ordinary multigaussian kriging honors the values of $\varphi(Y_{\mathbf{x}})$ at the data locations: at these locations, the ordinary kriging estimator matches the data values, whereas the kriging variance and Lagrange multiplier are equal to zero.
2. Because of the square root, Eq. 11 requires that $(\sigma_{\mathbf{x}}^{\text{OK}})^2 + 2\mu_{\mathbf{x}}$ is nonnegative. In general, this condi-

Fig. 1 Geometric interpretation of the simple and ordinary multigaussian kriging estimators

a
Gaussian variables with a unit variance

b
Gaussian variables with a unit variance

$Y_{\mathbf{x}}^{OK} + \sqrt{1-(s_{\mathbf{x}}^{OK})^2}\, T$

sum of weights = 1

c
Gaussian variables with a unit variance

sum of weights = 1

tion is fulfilled, since the variance of the ordinary kriging estimator (weighted average of the data) is usually smaller than the prior variance, i.e. $(s_{\mathbf{x}}^{OK})^2$ is lower than or equal to one (Eq. 13). Otherwise, one may replace ordinary kriging by another weighting of the normal scores data with a variance less than one,

a sufficient condition being that the weights are nonnegative and add to one to ensure unbiasedness, see Barnes and Johnson (1984), Herzfeld (1989) and Deutsch (1996).

3. The ordinary multigaussian kriging estimator is globally unbiased but not conditionally unbiased. In general, one has (Appendix A):

$$E\left\{\varphi(Y_{\mathbf{x}})|[\varphi(Y_{\mathbf{x}})]^{\mathrm{oMK}}\right\} \neq [\varphi(Y_{\mathbf{x}})]^{\mathrm{oMK}}. \tag{15}$$

As mentioned before (Eq. 6), any conditionally unbiased estimator of $\varphi(Y_{\mathbf{x}})$ converges to its prior expectation when moving away from the data. Therefore, to avoid this convergence, one must accept the presence of a conditional bias.

4. For the estimation purpose, everything occurs as if the posterior distribution of the unknown value $Y_{\mathbf{x}}$ were Gaussian, with mean equal to the ordinary kriging and variance the ordinary kriging variance plus twice the Lagrange multiplier (Eq. 11). This mathematically consistent distribution implies that the estimations do not violate order relations, for instance the estimation of a positive function is always positive or the estimation of an indicator function (Eq. 1) decreases when the threshold increases. However, this (pseudo) posterior distribution differs from the true one, for which the first- and second-order moments are the simple kriging and simple kriging variance (see Eq. 2).

In general, the variance of the pseudo posterior distribution of $Y_{\mathbf{x}}$ is lower than the simple kriging variance. Indeed, let λ_m be the weight assigned to the mean in the simple kriging estimator and $(\sigma_m^{\mathrm{OK}})^2$ the estimation variance of the unknown mean. The additivity theorem (Matheron 1971, p. 129) provides the following relationship:

$$(\sigma_{\mathbf{x}}^{\mathrm{OK}})^2 = (\sigma_{\mathbf{x}}^{\mathrm{SK}})^2 + \lambda_m^2 (\sigma_m^{\mathrm{OK}})^2. \tag{16}$$

Besides, the Lagrange multiplier introduced in the ordinary kriging system (Eq. 9) can be expressed as follows (Emery 2004, p. 411):

$$\mu_{\mathbf{x}} = -\lambda_m (\sigma_m^{\mathrm{OK}})^2. \tag{17}$$

Hence the variance of the pseudo posterior distribution of $Y_{\mathbf{x}}$ is

$$(\sigma_{\mathbf{x}}^{\mathrm{OK}})^2 + 2\mu_{\mathbf{x}} = (\sigma_{\mathbf{x}}^{\mathrm{SK}})^2 + \lambda_m (\lambda_m - 2) (\sigma_m^{\mathrm{OK}})^2. \tag{18}$$

Usually the weight of the mean λ_m is positive and less than 2, so the dispersion of the pseudo posterior distribution is smaller than the one of the true posterior distribution. This entails that the ordinary multigaussian kriging approach is not suitable for assessing the local uncertainty on the unsampled values of the regionalized variable, e.g. by deriving confidence intervals from the pseudo posterior distribution.

A geometric interpretation of multigaussian kriging

Equations 4 and 12 can be interpreted from a geometric point of view (Fig. 1). To simplify, suppose that the mean m is equal to zero and consider the vector space spanned by the Gaussian variables at locations $\mathbf{x}$ and $\{\mathbf{x}_\alpha, \ \alpha = 1,..., n\}$. This space is provided with a scalar product equal to the covariance operator. For visualization purposes the drawing is restricted to the case $n = 2$. The unit sphere represents all the Gaussian random variables with a unit variance that can be obtained by linear combinations of the three variables $Y_{\mathbf{x}}, Y_{\mathbf{x}_1}, Y_{\mathbf{x}_2}$. Let Ψ be an element of this sphere, Ψ^* its orthogonal projection onto the plane H spanned by the data $Y_{\mathbf{x}_1}, Y_{\mathbf{x}_2}$ and $\Psi_\perp = \Psi - \Psi^*$ the residual, which is orthogonal to H (Fig. 1a). Since $\varphi(Y_{\mathbf{x}})$ and $\varphi(\Psi)$ have the same expected value, an unbiased estimator of $\varphi(Y_{\mathbf{x}})$ is obtained by putting

$$[\varphi(Y_{\mathbf{x}})]^* = E\{\varphi(\Psi)|\Psi^*\} \tag{19}$$

For instance, the orthogonal projection of $Y_{\mathbf{x}}$ onto H is its simple kriging (Journel and Huijbregts 1978, p. 559). It always falls inside the sphere and it is therefore possible to find a Gaussian variable orthogonal to H (the simple kriging error) such that the sum is located on the sphere (Eqs. 2, 4):

$$\begin{cases} \Psi^* = Y_{\mathbf{x}}^{\mathrm{SK}} \\ \Psi_\perp = \sigma_{\mathbf{x}}^{\mathrm{SK}} T \\ \Psi = Y_{\mathbf{x}}. \end{cases} \tag{20}$$

Ordinary kriging is the orthogonal projection of $Y_{\mathbf{x}}$ onto the line that joins the two data (this line represents the constraint that the kriging weights add to one). It may occasionally fall outside the unit sphere (Fig. 1c): in this case, the variance of the ordinary kriging estimator is greater than one and no independent random variable can be added to come back to the sphere. Otherwise, one has (Eq. 12 and Fig. 1b):

$$\begin{cases} \Psi^* = Y_{\mathbf{x}}^{\mathrm{OK}} \\ \Psi_\perp = \sqrt{1 - (s_{\mathbf{x}}^{\mathrm{OK}})^2} T \\ \Psi = Y_{\mathbf{x}}^{\mathrm{OK}} + \sqrt{1 - (s_{\mathbf{x}}^{\mathrm{OK}})^2} T. \end{cases} \tag{21}$$

Example: lognormal kriging

An interesting example is the case when φ is an exponential function, which amounts to estimating a lognormal variable:

$$\varphi(Y_{\mathbf{x}}) = \exp(\sigma Y_{\mathbf{x}}) \text{ with } \sigma \in R. \tag{22}$$

After simplification, the simple and ordinary multigaussian kriging estimators (Eqs. 3, 11) are found to

coincide with the so-called simple and ordinary lognormal kriging:

$$[\exp(\sigma Y_{\mathbf{x}})]^{\text{sMK}} = \exp\left(\sigma Y_{\mathbf{x}}^{\text{SK}} + \frac{\sigma^2 (\sigma_{\mathbf{x}}^{\text{SK}})^2}{2}\right)$$
$$[\exp(\sigma Y_{\mathbf{x}})]^{\text{oMK}} = \exp\left({}_{\mathbf{x}}^{\text{OK}} + \frac{\sigma^2 (\sigma_{\mathbf{x}}^{\text{OK}})^2}{2} + \sigma^2 \mu_{\mathbf{x}}\right). \tag{23}$$

Lognormal kriging has been extensively studied in the geostatistical literature, mainly in the scope of ore reserve evaluation problems (Matheron 1974; Parker et al. 1979; Rendu 1979; Journel 1980; Dowd 1982; Rivoirard 1990). So far, it was considered an exceptional case where an ordinary kriging of the normal scores data could be used without provoking a bias (Rivoirard 1994, p. 71; Chilès and Delfiner 1999, p. 382). However, the previous statements about ordinary multigaussian kriging show that the incorporation of a constraint on the sum of the kriging weights is not specific to the lognormal model.

Precision of multigaussian kriging

The unbiasedness (accuracy) of multigaussian kriging does not entail that this estimator is precise, as the estimation errors may be highly dispersed and only compensate in average. The precision of an estimator is usually quantified by calculating the variance of the estimation error. For instance, concerning simple multigaussian kriging, this variance is expressed as follows (Eq. 7):

$$\text{var}\left\{\varphi(Y_{\mathbf{x}}) - [\varphi(Y_{\mathbf{x}})]^{\text{sMK}}\right\}$$
$$= \text{var}\{\varphi(Y_{\mathbf{x}})\} - \text{var}\left\{[\varphi(Y_{\mathbf{x}})]^{\text{sMK}}\right\}. \tag{24}$$

To go further and get a workable analytical expression of this variance, it is useful to expand the estimator into Hermite polynomials.

Expansion of the multigaussian kriging estimator into Hermite polynomials

The normalized Hermite polynomials $\{H_p, \; p \in N\}$ (Hochstrasser 1972) form an orthonormal basis with respect to the standard bivariate Gaussian distribution, that is:

1. Any function of $L_2(R,g)$ (i.e. the space of functions that are square-integrable with respect to the measure defined by the standard Gaussian density g) can be expanded into Hermite polynomials, i.e. there exists a unique set of scalar coefficients $\{\varphi_p(m), \; p \in N\}$ such that:

$$\forall y \in R, \varphi(m + y) = \sum_{p=0}^{+\infty} \varphi_p(m) H_p(y). \tag{25}$$

2. If $\{Y, Y'\}$ has a standard bigaussian distribution with correlation coefficient r, then for any positive integers p and q:

$$\begin{cases} E\{H_p(Y)\} = 0 \\ \text{cov}\{H_p(Y), H_q(Y')\} = \begin{vmatrix} 0 & \text{if } p \neq q \\ r^p & \text{otherwise.} \end{vmatrix} \end{cases} \tag{26}$$

From these properties, the following expansions can be established (Emery 2005b, pp. 299–305):

– Transfer function to estimate:

$$\varphi(Y_{\mathbf{x}}) = \sum_{p=0}^{+\infty} \varphi_p(m) H_p(Y_{\mathbf{x}} - m). \tag{27}$$

– Simple multigaussian kriging:

$$[\varphi(Y_{\mathbf{x}})]^{\text{sMK}} = \sum_{p=0}^{+\infty} \varphi_p(m) (s_{\mathbf{x}}^{\text{SK}})^p H_p\left(\frac{Y_{\mathbf{x}}^{\text{SK}} - m}{s_{\mathbf{x}}^{\text{SK}}}\right), \tag{28}$$

where $(s_{\mathbf{x}}^{\text{SK}})^2$ is the variance of the simple kriging estimator, which is equal to the prior variance minus the simple kriging variance (Chilès and Delfiner 1999, p. 162):

$$(s_{\mathbf{x}}^{\text{SK}})^2 = \text{var}(Y_{\mathbf{x}}^{\text{SK}}) = 1 - (\sigma_{\mathbf{x}}^{\text{SK}})^2. \tag{29}$$

The convergence rate of the series in Eq. 28 is faster than the one in Eq. 27, because the coefficients $\{\varphi_p(m), \; p \in N\}$ are multiplied by the successive terms of a geometric series with common ratio less than one. Consequently, Eq. 28 can be used to calculate the simple multigaussian kriging estimator by truncating the summation to a high order (say, $P_{\max} = 100$) instead of resorting to a numerical integration of Eq. 3 (Emery 2005b, p. 300).

– Ordinary multigaussian kriging:

$$[\varphi(Y_{\mathbf{x}})]^{\text{oMK}} = \sum_{p=0}^{+\infty} \varphi_p(m) (s_{\mathbf{x}}^{\text{OK}})^p H_p\left(\frac{Y_{\mathbf{x}}^{\text{OK}} - m}{s_{\mathbf{x}}^{\text{OK}}}\right). \tag{30}$$

Since the estimator does not depend on the mean m (Eq. 11), one also has

$$[\varphi(Y_{\mathbf{x}})]^{\text{oMK}} = \sum_{p=0}^{+\infty} \varphi_p(0) (s_{\mathbf{x}}^{\text{OK}})^p H_p\left(\frac{Y_{\mathbf{x}}^{\text{OK}}}{s_{\mathbf{x}}^{\text{OK}}}\right). \tag{31}$$

Again, this equation can be used to calculate the ordinary multigaussian kriging estimator, by truncating the expansion to a high order. It is also interesting for establishing the conditions under which the estimator can be defined. Indeed, the expansion converges if and only if the sum of the squares of $\{\varphi_p(0) (s_{\mathbf{x}}^{\text{OK}})^p, \; p \in N\}$ is finite. A sufficient condition is that $s_{\mathbf{x}}^{\text{OK}}$ is less than or equal to one, a situation that has been mentioned earlier, but this is not a necessary condition. For instance, Eq. 31 converges for any value of $s_{\mathbf{x}}^{\text{OK}}$ if φ is a polyno-

mial (finite expansion) or an exponential function (ordinary lognormal kriging). In contrast, if φ is an indicator function (Eq. 1), the expansion diverges as soon as $s_\mathbf{x}^{OK}$ is greater than one.

Expression of the estimation variances

The calculation of the estimation variances is based on the previous expansions and on the orthonormality of the Hermite polynomials for the bigaussian distribution (Eq. 26). It comes (proof in Appendix B):

– Simple multigaussian kriging variance:

$$\mathrm{var}\{\varphi(Y_\mathbf{x}) - [\varphi(Y_\mathbf{x})]^{sMK}\}$$
$$= \sum_{p=1}^{+\infty} \varphi_p^2(m) \{1 - [1 - (\sigma_\mathbf{x}^{SK})^2]^p\}.$$

– Ordinary multigaussian kriging variance:

$$\mathrm{var}\{\varphi(Y_\mathbf{x}) - [\varphi(Y_\mathbf{x})]^{oMK}\}$$
$$= \sum_{p=1}^{+\infty} \varphi_p^2(m)\{1 + [1 - (\sigma_\mathbf{x}^{OK})^2 - 2\mu_\mathbf{x}]^p - 2[1 - (\sigma_\mathbf{x}^{OK})^2 - \mu_\mathbf{x}]^p\}.$$
$$(33)$$

In practice, Eqs. 32 and 33 can be calculated numerically by truncating the expansions to a high order. The estimation variances explicitly depend on the value of the mean (m); if this mean is unknown, an approximation consists in replacing m by its optimal estimate or by zero (mean value in the ideal multigaussian model). In contrast, the previous variances are not conditional, in the sense that they do not depend on the data values. It is also possible to define a conditional variance, which is a more realistic measure of the uncertainty on the value of $\varphi(Y_\mathbf{x})$:

$$\mathrm{var}\{\varphi(Y_\mathbf{x})|\mathrm{data}\} = [\varphi^2(Y_\mathbf{x})]^{sMK} - \{[\varphi(Y_\mathbf{x})]^{sMK}\}^2. \quad (34)$$

This variance can be calculated provided that the mean is known. Its expected value is the non-conditional variance given in Eqs. 24 and 32. As an example, let us consider again the case where φ is an exponential function (Eq. 22); the Hermitian expansion of such a function can be found in Chilès and Delfiner (1999, p. 641). After simplification, the following non-conditional and conditional estimation variances are found:

$$\mathrm{var}\{\exp(\sigma Y_\mathbf{x}) - [\exp(\sigma Y_\mathbf{x})]^{sMK}\}$$
$$= \mathrm{e}^{2\sigma(m+\sigma)}\{1 - \mathrm{e}^{-\sigma^2(\sigma_\mathbf{x}^{SK})^2}\}, \quad (35)$$

$$\mathrm{var}\{\exp(\sigma Y_\mathbf{x}) - [\exp(\sigma Y_\mathbf{x})]^{oMK}\}$$
$$= e^{2\sigma(m+\sigma)}\{1 + e^{-\sigma^2[(\sigma_\mathbf{x}^{OK})^2 + \mu_\mathbf{x}]}(e^{-\sigma^2\mu_\mathbf{x}} - 2)\} \quad (36)$$

and

$$\mathrm{var}\{\exp(\sigma Y_\mathbf{x})|\mathrm{data}\} = \mathrm{e}^{2\sigma Y_\mathbf{x}^{SK} + \sigma^2(\sigma_\mathbf{x}^{SK})^2}\{\mathrm{e}^{\sigma^2(\sigma_\mathbf{x}^{SK})^2} - 1\}. \quad (37)$$

These formulae coincide with the expressions given by Rendu (1979, pp. 417–419), Journel (1980, pp. 291–295) and Dowd (1982, pp. 482–84). Note that the conditional variance is proportional to the square of the simple lognormal kriging estimator, a feature known as "proportional effect".

On the optimality of multigaussian kriging

Known mean

Simple multigaussian kriging coincides with the conditional expectation estimator in the multigaussian framework, which is known to minimize the estimation variance among all the estimators constructed from the data (Chilès and Delfiner 1999, p. 14). Hence it constitutes the "optimal" estimator if the mean value is known, provided of course that the multigaussian hypothesis is suited to the data under study.

Unknown mean

Unlike simple multigaussian kriging, ordinary multigaussian kriging is not a conditional expectation estimator and may not minimize the estimation variance. The reader will find in Appendix C some elements on the construction of a disjunctive-type estimator that is unbiased and theoretically more precise than ordinary multigaussian kriging. The idea is to seek an estimator that minimizes the error variance of each term of the Hermitian expansion of $\varphi(Y_\mathbf{x})$ (Eq. 27), by putting:

$$[\varphi(Y_\mathbf{x})]^* = \sum_{p=0}^{+\infty} \varphi_p(0)\,(s_{\mathbf{x},p}^*)^p H_p\left(\frac{Y_{\mathbf{x},p}^*}{s_{\mathbf{x},p}^*}\right), \quad (38)$$

where $\{Y_{\mathbf{x},p}^*, p \in N\}$ is a set of weighted averages of the normal scores data whose weights add to one, and $\{(s_{\mathbf{x},p}^*)^2, p \in N\}$ their respective variances.

To compare the performance of this disjunctive estimator with the one of simple and ordinary multigaussian kriging, we propose to examine a few kriging configurations. More precisely, let us consider three data in a two-dimensional space and four locations to estimate, as shown in Fig. 2.

In this exercise, the correlogram of the Gaussian random field $\{Y_\mathbf{x}, \mathbf{x} \in R^2\}$ is supposed to be an isotropic exponential model with practical range a and sill $C = 0.9$, plus a nugget effect with sill $1 - C = 0.1$. Two values of the range are tested: $a = 2$ and $a = 10$. For both range values and each location to estimate, the estimation variances of the first ten Hermite polynomials are calculated, corresponding to simple multigaussian kriging (solid lines in Fig. 3), ordinary multigaussian kriging (circles in Fig. 3) and the disjunctive estimator given in

Fig. 2 Two-dimensional kriging configuration with three data and four locations to estimate
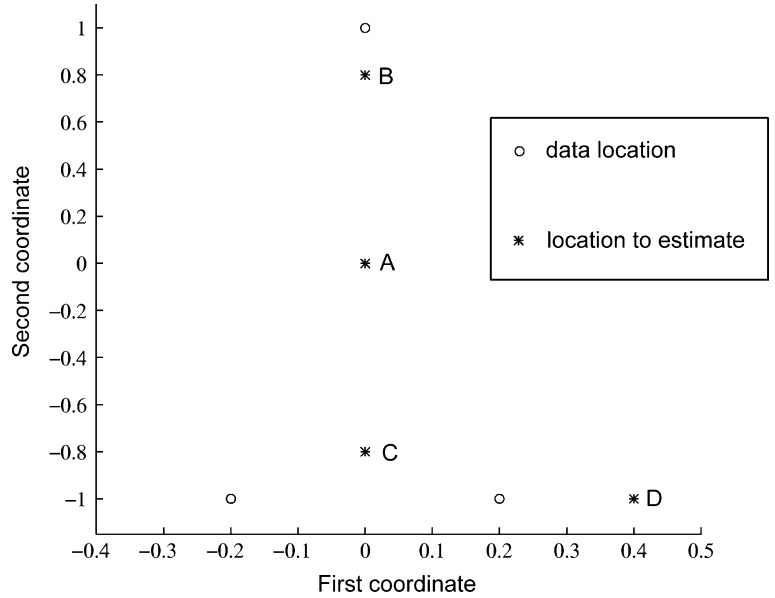
Eq. 38 (dotted lines in Fig. 3). In the analyzed configurations, the latter improves the estimation variance of ordinary multigaussian kriging up to 5% (especially for the polynomials of degrees 3–8 at locations B and D) and therefore constitutes a worthy alternative to it. In practice however, ordinary multigaussian kriging is much simpler to calculate and may be preferred by practitioners. The advantages of the disjunctive estimator vanish when

1. The nugget effect of the correlogram model is important: this situation leads to an equal weighting of the normal scores data for both the disjunctive estimator and ordinary multigaussian kriging;
2. The data are abundant or the location to estimate is close to a datum. Simple kriging is then close to ordinary kriging (the weight of the mean is low in the simple kriging estimator), hence ordinary multigaussian kriging is almost optimal;
3. The location to estimate is distant from any datum. In this case, for any integer p, the optimal weighting in Eq. 38 is the ordinary kriging of the data (proof in Appendix C), hence the disjunctive estimator coincides with ordinary multigaussian kriging.

Misspecified mean

In this last subsection, we examine the robustness of simple multigaussian kriging to a misspecification of the mean value and compare its performance to ordinary multigaussian kriging. For sake of simplicity, the analysis is restricted to the lognormal case, for which analytical formulae can be derived. Suppose that the mean value of the normal scores data is wrongly specified by the user, who assumes a mean equal to m' instead of m. In the following, we will assume that m' is the optimal estimator of the true unknown mean, obtained by ordinary kriging from the normal scores data. Because of

the additivity relationship (Matheron 1971, p. 129), using m' instead of m amounts to substituting ordinary kriging for simple kriging in the traditional lognormal kriging estimator (Eq. 23):

$$[\exp(\sigma Y_{\mathbf{x}})]^* = \exp\left(\sigma Y_{\mathbf{x}}^{\mathrm{OK}} + \frac{\sigma^2 (\sigma_{\mathbf{x}}^{\mathrm{SK}})^2}{2}\right). \tag{39}$$

This kind of estimator has been proposed by Goovaerts (1997, p. 282); however, in general it is not unbiased. Its quality can be characterized by the associated mean squared error (denoted by $\mathrm{MSE}_{\mathrm{SMK}}$ in the following), a measure that accounts for both the error mean (accuracy) and error variance (precision). When $\mathbf{x}$ coincides with a data location, this mean squared error is zero because the estimator honors the data values. In the following, we examine the opposite case when $Y_{\mathbf{x}}$ is correlated with none of the data. After simplification, the following mean squared error is found:

$$\mathrm{MSE}_{\mathrm{SMK}} = e^{2\sigma(m+\sigma)}\{1 + e^{\frac{1}{2}\sigma^2 (\sigma_m^{\mathrm{OK}})^2 - \sigma^2}[e^{\frac{3}{2}\sigma^2 (\sigma_m^{\mathrm{OK}})^2} - 2]\}, \tag{40}$$

where $(\sigma_m^{\mathrm{OK}})^2$ is the optimal estimation variance of the unknown mean. This quantity has to be compared to the mean squared error of ordinary lognormal kriging (Eq. 36). Under the same conditions as above ($Y_{\mathbf{x}}$ uncorrelated with the data), the latter becomes:

$$\mathrm{MSE}_{\mathrm{OMK}} = e^{2\sigma(m+\sigma)}\{1 + e^{-\sigma^2}[e^{\sigma^2(\sigma_m^{\mathrm{OK}})^2} - 2]\}. \tag{41}$$

The performances of the two estimators (simple lognormal kriging with a misspecified mean and ordinary lognormal kriging) can be compared through the ratio

$$\frac{\mathrm{MSE}_{\mathrm{SMK}}}{\mathrm{MSE}_{\mathrm{OMK}}} = \frac{1 + e^{\frac{1}{2}\sigma^2 (\sigma_m^{\mathrm{OK}})^2 - \sigma^2}[e^{\frac{3}{2}\sigma^2 (\sigma_m^{\mathrm{OK}})^2} - 2]}{1 + e^{-\sigma^2}[e^{\sigma^2 (\sigma_m^{\mathrm{OK}})^2} - 2]}. \tag{42}$$

Fig. 3 Estimation variances of the first ten Hermite polynomials associated with simple and ordinary multigaussian kriging and the disjunctive-type estimator given in Eq. 38
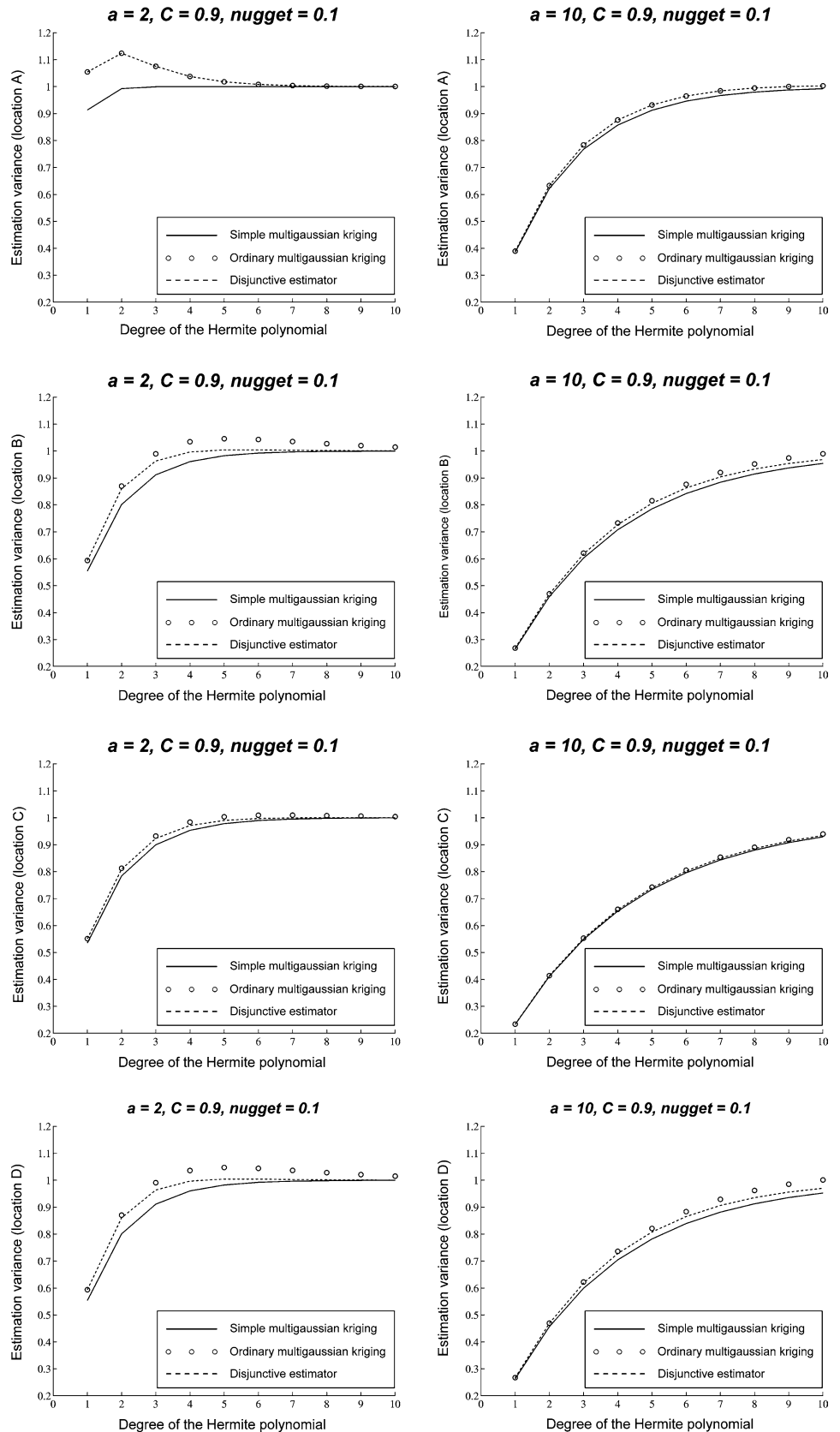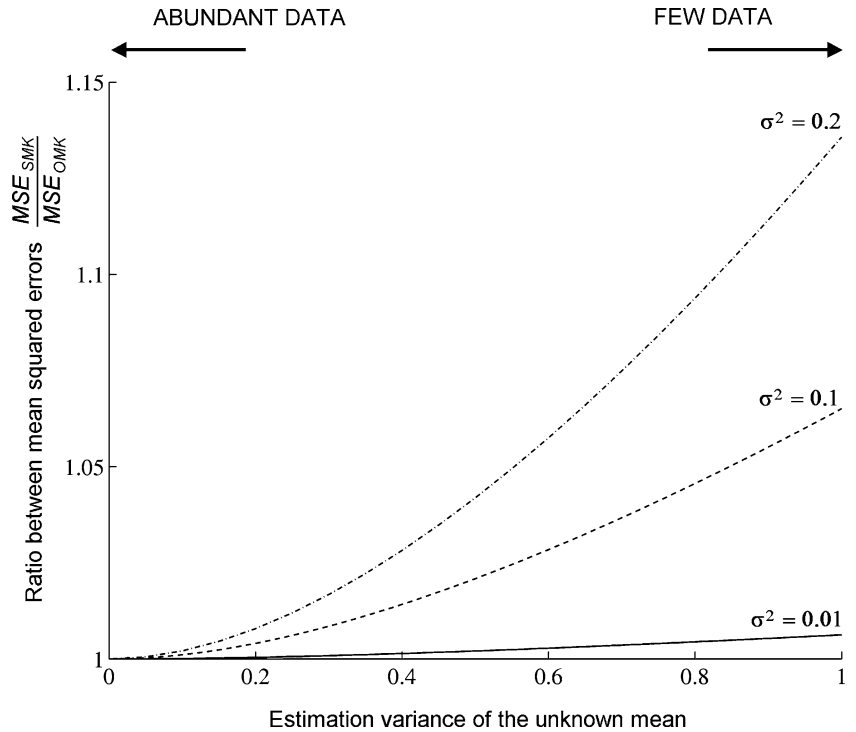
Fig. 4 Ratio of the mean squared errors between simple lognormal kriging with a misspecified mean and ordinary lognormal kriging. A ratio greater than one indicates that the former estimator is less precise than the latter

As shown in Fig. 4 for several values of σ^2, this ratio is always greater than one, which indicates that, in case of using an estimated mean instead of the true mean, simple lognormal kriging produces a greater mean squared error than ordinary lognormal kriging. The latter should therefore be preferred to the former, inasmuch as its implementation is straightforward and entails no bias and better precision. The difference between both estimators narrows when the estimation variance of the mean is close to zero (the data are abundant) or when the logarithmic variance σ^2 is low (in this case, the function to estimate is almost linear).

Although they have been established in a specific case (lognormal kriging), these results indicate that simple multigaussian kriging may not be robust to misspecifications of the mean value of the normal scores data, especially if the function to estimate is highly nonlinear, and give poorer results than ordinary multigaussian kriging.

Conclusions

The multigaussian approach offers a simple framework for assessing a point-support transfer function of a regionalized variable. Contrarily to other nonlinear geostatistical methods such as indicator and disjunctive kriging, multigaussian kriging takes advantage of the multivariate distribution of the available data and does not lead to order-relation violations, since the estimator is based on a mathematically consistent posterior distribution. It can also account for an unknown mean of the normal scores data and therefore be robust to local variations of this mean over the domain of interest.

The simple and ordinary multigaussian kriging estimators, as well as the associated estimation variances, can be expressed and calculated thanks to expansions into Hermite polynomials. Additionally, such expansions allow one to define a disjunctive-type estimator that minimizes the estimation variance when the Gaussian field has an unknown mean and is theoretically more precise than ordinary multigaussian kriging. Two possible extensions of the approach presented in this paper are:

- *Multivariate problems*: by assuming that all the regionalized variables can be modeled by jointly-Gaussian random fields, the multigaussian kriging formalism can be generalized by substituting a (simple or ordinary) cokriging for the (simple or ordinary) kriging;
- *Change-of-support problems*: these problems are important in mining engineering and environmental sciences; they can be tackled in the scope of the discrete Gaussian model (Rivoirard 1994, p. 88; Chilès and Delfiner 1999, p. 438) instead of the point-support multigaussian model.

Appendix A

This appendix analyses the conditional bias of the ordinary multigaussian kriging estimator (Eq. 11). To

quantify this bias, let us calculate the regression of $\varphi(Y_\mathbf{x})$ upon $[\varphi(Y_\mathbf{x})]^{\text{oMK}}$. Since the latter is a function of the ordinary kriging estimator (to simplify, we suppose that this is a one-to-one function), conditioning to $[\varphi(Y_\mathbf{x})]^{\text{oMK}}$ amounts to conditioning to $Y_\mathbf{x}^{\text{OK}}$:

$$E\{\varphi(Y_\mathbf{x})|[\varphi(Y_\mathbf{x})]^{\text{oMK}}\} = E\{\varphi(Y_\mathbf{x})|Y_\mathbf{x}^{\text{OK}}\}. \tag{43}$$

The pair $\{Y_\mathbf{x} - m, (Y_\mathbf{x}^{\text{OK}} - m)/s_\mathbf{x}^{\text{OK}}\}$ has a standard bigaussian distribution with correlation coefficient (Eqs. 8, 10)

$$r_\mathbf{x}^{\text{OK}} = \frac{1}{s_\mathbf{x}^{\text{OK}}} \sum_{\alpha=1}^{n} \lambda_\alpha^{\text{OK}} \rho(\mathbf{x}_\alpha, \mathbf{x}) = \frac{1 - (\sigma_\mathbf{x}^{\text{OK}})^2 - \mu_\mathbf{x}}{s_\mathbf{x}^{\text{OK}}}. \tag{44}$$

Hence, one can write (Rivoirard 1994, p. 50):

$$Y_\mathbf{x} = m + \frac{r_\mathbf{x}^{\text{OK}}}{s_\mathbf{x}^{\text{OK}}}(Y_\mathbf{x}^{\text{OK}} - m) + \sqrt{1 - (r_\mathbf{x}^{\text{OK}})^2}\, U, \tag{45}$$

where U is a standard Gaussian variable independent of $Y_\mathbf{x}^{\text{OK}}$. This identity allows one to calculate the regression curve between the true and estimated values of $\varphi(Y_\mathbf{x})$ (Eq. 43):

$$E\{\varphi(Y_\mathbf{x})|[\varphi(Y_\mathbf{x})]^{\text{oMK}}\}$$
$$= \int \varphi\left(m + \frac{r_\mathbf{x}^{\text{OK}}}{s_\mathbf{x}^{\text{OK}}}(Y_\mathbf{x}^{\text{OK}} - m) + \sqrt{1 - (r_\mathbf{x}^{\text{OK}})^2}\, u\right) g(u)\, du. \tag{46}$$

A comparison with Eq. 11 shows that, in general, a conditional bias is present (Eq. 15), unless $r_\mathbf{x}^{\text{OK}} = s_\mathbf{x}^{\text{OK}}$: in this case, the Lagrange multiplier $\mu_\mathbf{x}$ is equal to zero because of Eqs. 13 and 44, and ordinary multigaussian kriging coincides with simple multigaussian kriging. However, this is a very specific circumstance as it implies that the weight of the mean is equal to zero in the simple kriging system (Eq. 17).

Appendix B

In this appendix, we establish the analytical expressions of the estimation variances associated with multigaussian kriging. To make the demonstration more general, let us consider a weighted average of the normal scores data and mean value that estimates $Y_\mathbf{x}$ without bias:

$$Y_\mathbf{x}^* = \sum_{\alpha=1}^{n} \lambda_\alpha Y_{\mathbf{x}_\alpha} + \left(1 - \sum_{\alpha=1}^{n} \lambda_\alpha\right) m. \tag{47}$$

The variance of $Y_\mathbf{x}^*$ and its covariance with $Y_\mathbf{x}$ are:

$$\begin{cases} \text{var}(Y_\mathbf{x}^*) = (s_\mathbf{x}^*)^2 = \sum_{\alpha=1}^{n} \sum_{\beta=1}^{n} \lambda_\alpha \lambda_\beta\, \rho(\mathbf{x}_\alpha, \mathbf{x}_\beta) \\ \text{cov}(Y_\mathbf{x}, Y_\mathbf{x}^*) = r_\mathbf{x}^* s_\mathbf{x}^* = \sum_{\alpha=1}^{n} \lambda_\alpha\, \rho(\mathbf{x}_\alpha, \mathbf{x}) \end{cases} \tag{48}$$

so that $\{Y_\mathbf{x} - m, (Y_\mathbf{x}^* - m)/s_\mathbf{x}^*\}$ is a standard bigaussian pair with correlation coefficient $r_\mathbf{x}^*$.

Let us now define an unbiased estimator of $\varphi(Y_\mathbf{x})$ as:

$$\begin{aligned} [\varphi(Y_\mathbf{x})]^* &= \int \varphi\left(Y_\mathbf{x}^* + \sqrt{1 - (s_\mathbf{x}^*)^2}\, t\right) g(t)\, dt \\ &= \sum_{p=0}^{+\infty} \varphi_p(m)\, (s_\mathbf{x}^*)^p H_p\left(\frac{Y_\mathbf{x}^* - m}{s_\mathbf{x}^*}\right) \end{aligned} \tag{49}$$

The estimation variance of the estimator defined in Eq. 49 is found by considering the Hermitian expansions of the transfer function (Eq. 27) and by using the orthonormality of the Hermite polynomials for the bigaussian distribution (Eq. 26):

$$\begin{aligned} &\text{var}\{\varphi(Y_\mathbf{x}) - [\varphi(Y_\mathbf{x})]^*\} \\ &= \text{var}\{\varphi(Y_\mathbf{x})\} + \text{var}\{[\varphi(Y_\mathbf{x})]^*\} - 2\, \text{cov}\{\varphi(Y_\mathbf{x}), [\varphi(Y_\mathbf{x})]^*\} \\ &= \sum_{p=1}^{+\infty} \varphi_p^2(m)\, \{1 + (s_\mathbf{x}^*)^{2p} - 2\, (r_\mathbf{x}^* s_\mathbf{x}^*)^p\}. \end{aligned}$$
$$\tag{50}$$

The estimation variances of the simple and ordinary multigaussian kriging estimators (Eqs. 32, 33) are particular cases of this formula, obtained by using the simple and ordinary kriging weights in Eq. 48.

Appendix C

This appendix aims at obtaining an "optimal" unbiased estimator of $\varphi(Y_\mathbf{x})$ in case of an unknown mean. By convention, the criterion for optimality is the minimization of the estimation variance. Equation 49 provides a general form of an unbiased estimator of $\varphi(Y_\mathbf{x})$. Suppose one does not use ordinary kriging but another weighted average of the normal scores data, such that the weights add to one:

$$Y_\mathbf{x}^* = \sum_{\alpha=1}^{n} \lambda_\alpha Y_{\mathbf{x}_\alpha} \quad \text{with} \quad \sum_{\alpha=1}^{n} \lambda_\alpha = 1. \tag{51}$$

Since $Y_\mathbf{x}^*$ does no longer depend on the mean value m, the estimator in Eq. 49 can also be written as follows:

$$[\varphi(Y_\mathbf{x})]^* = \sum_{p=0}^{+\infty} \varphi_p(0)(s_\mathbf{x}^*)^p H_p\left(\frac{Y_\mathbf{x}^*}{s_\mathbf{x}^*}\right). \tag{52}$$

It is not obvious that ordinary kriging minimizes the estimation variance (Eq. 50) among all the weighted averages of the normal scores data with total weight equal to one. Actually, this is the case for linear functions of $Y_\mathbf{x}$, but not for any function φ. Matheron (1974, p. 30) examined the case of an exponential function (lognormal model) and proposed an algorithm to obtain the optimal weighting for $Y_\mathbf{x}^*$, i.e. to find the weighted average that minimizes the estimation variance of the lognormal estimator.

A closer look at Eq. 50 shows that the best choice of the weighted average depends on the coefficients $\{\varphi_p(m), p \in N\}$ and that one can construct a more general estimator which minimizes each term of the estimation variance by putting (Eq. 38):

$$[\varphi(Y_{\mathbf{x}})]^* = \sum_{p=0}^{+\infty} \varphi_p(0)(s_{\mathbf{x},p}^*)^p H_p\left(\frac{Y_{\mathbf{x},p}^*}{s_{\mathbf{x},p}^*}\right) \qquad (53)$$

for a set of weighted averages $\{Y_{\mathbf{x},p}^* = \sum_{\alpha=1}^{n} \lambda_{\alpha,p} Y_{\mathbf{x}_\alpha}, p \in N\}$ to be determined.

The unbiasedness of this estimator can be established by recalling that, for any Gaussian random variable Y with mean m and variance s^2, one has (Emery 2005b, p. 319):

$$E\left\{s^p H_p\left(\frac{Y}{s}\right)\right\} = \frac{(-m)^p}{\sqrt{p!}}. \qquad (54)$$

Consequently, the disjunctive-type estimator in Eq. 53 has the same expected value as ordinary multigaussian kriging (Eq. 31), which is the same as the expected value of the transfer function to estimate:

$$E\{[\varphi(Y_{\mathbf{x}})]^*\} = E\{[\varphi(Y_{\mathbf{x}})]^{\mathrm{oMK}}\} = E\{[\varphi(Y_{\mathbf{x}})]\}. \qquad (55)$$

The calculation of the estimation variance is more tricky, as the exact expression of this variance depends on the unknown mean value m. To break the deadlock, one has to choose a model (with a specified mean value) and calculate the estimation variance in the framework of this model. Note that, in contrast, the unbiasedness condition (Eq. 55) is independent of this model since the expected value of the estimation error is zero, regardless of the mean value. Here, we will use the "ideal" multigaussian model, for which the normal scores data have a zero mean. In this case, the estimation variance of the Hermite polynomial of degree p, which contributes to the p-th term of Eq. 50, is:

$$\mathrm{var}\{H_p(Y_{\mathbf{x}}) - [H_p(Y_{\mathbf{x}})]^*\} = 1 + (s_{\mathbf{x},p}^*)^{2p} - 2(r_{\mathbf{x},p}^* s_{\mathbf{x},p}^*)^p \qquad (56)$$

and the minimization under the restriction on the sum of the weights (Eq. 51) leads to the following system of nonlinear equations:

$$\begin{cases} \left[\sum_{\beta,\delta=1}^{n} \lambda_{\beta,p} \lambda_{\delta,p} \rho(\mathbf{x}_\beta, \mathbf{x}_\delta)\right]^{p-1} \sum_{\beta=1}^{n} \lambda_{\beta,p} \rho(\mathbf{x}_\alpha, \mathbf{x}_\beta) + \mu_p \\ = \left[\sum_{\beta=1}^{n} \lambda_{\beta,p} \rho(\mathbf{x}_\beta, \mathbf{x})\right]^{p-1} \rho(\mathbf{x}_\alpha, \mathbf{x}) \quad \forall \alpha = 1, ..., n \\ \sum_{\beta=1}^{n} \lambda_{\beta,p} = 1. \end{cases} \qquad (57)$$

In practice, this system can be solved by iterations. The initial guess $\{\lambda_{\beta,p}^{(0)}, \beta = 1,..., n\}$ may be the solution of the ordinary kriging system (Eq. 9). At step k, one solves the linear system

$$\begin{cases} \sum_{\beta=1}^{n} \lambda_{\beta,p}^{(k)} \rho(\mathbf{x}_\alpha, \mathbf{x}_\beta) + v_p^{(k)} \\ = \left[\dfrac{\sum_{\beta=1}^{n} \lambda_{\beta,p}^{(k-1)} \rho(\mathbf{x}_\beta, \mathbf{x})}{\sum_{\beta,\delta=1}^{n} \lambda_{\beta,p}^{(k-1)} \lambda_{\delta,p}^{(k-1)} \rho(\mathbf{x}_\beta, \mathbf{x}_\delta)}\right]^{p-1} \rho(\mathbf{x}_\alpha, \mathbf{x}) \quad \forall \alpha = 1, ..., n \\ \sum_{\beta=1}^{n} \lambda_{\beta,p}^{(k)} = 1. \end{cases}$$
$$(58)$$

This iterative algorithm is based on a fixed-point method. It is quite easy to implement but may not necessarily converge, or converge slowly. Alternative iterative algorithms can be used to solve system Eq. 57, see for instance Ortega and Rheinboldt (1970) and Dennis and Schnabel (1983).

As a particular case, if the distance from $\mathbf{x}$ to any of the data locations $\{\mathbf{x}_\alpha, \alpha = 1,..., n\}$ is greater than the range of the correlogram model, then system Eq. 58 is the same as the ordinary kriging system of the unknown mean (Matheron 1971, p. 128), or equivalently the ordinary kriging system of a location distant from all the data:

$$\begin{cases} \sum_{\beta=1}^{n} \lambda_{\beta,p}^{(k)} \rho(\mathbf{x}_\alpha, \mathbf{x}_\beta) + v_p^{(k)} = 0 \quad \forall \alpha = 1, ..., n \\ \sum_{\beta=1}^{n} \lambda_{\beta,p}^{(k)} = 1. \end{cases} \qquad (59)$$

This implies that, far from the data, the disjunctive-type estimator proposed in Eq. 53 coincides with the ordinary multigaussian kriging estimator. Note that both estimators are also the same at the data locations as they honor the values of the transfer function to estimate. As a consequence, the disjunctive estimator (Eq. 53) is a worthy alternative to ordinary multigaussian kriging only for "intermediate" locations, not too close nor too distant from the data.

References

Barnes RJ, Johnson TB (1984) Positive kriging. In: Verly G, David M, Journel AG, Maréchal A (eds) Geostatistics for natural resources characterization. Reidel, Dordrecht, pp 231–244

Chica-Olmo M, Luque-Espinar JA (2002) Applications of the local estimation of the probability distribution function in environmental sciences by kriging methods. Inverse Probl 18(1):25–36

Chilès JP, Delfiner P (1999) Geostatistics: modeling spatial uncertainty. Wiley, New York, p 695

Dennis JE, Schnabel RB (1983) Numerical methods for unconstrained optimization and nonlinear equations. Prentice-Hall (Prentice-Hall Series in Computational Mathematics), Englewood Cliffs, p 378

Deutsch CV (1996) Correcting for negative weights in ordinary kriging. Comput Geosci 22(7):765–773

Dowd PA (1982) Lognormal kriging—the general case. Math Geol 14(5):475–499

Emery X (2004) Testing the correctness of the sequential algorithm for simulating Gaussian random fields. Stoch Environ Res Risk Assess 18(6): 401–413. (DOI 10.1007/s00477-004-0211-7)

Emery X (2005a) Variograms of order ω: a tool to validate a bivariate distribution model. Math Geol 37(2):163–181. (DOI 10.1007/s11004-005-1307-4)

Emery X (2005b) Simple and ordinary multigaussian kriging for estimating recoverable reserves. Math Geol 37(3):295–319. (DOI 10.1007/s11004-005-1560-6)

Emery X (2006) Ordinary multigaussian kriging for mapping conditional probabilities of soil properties. Geoderma (in press). (DOI 10.1016/j.geoderma.2005.04.019)

Goovaerts P (1997) Geostatistics for natural resources evaluation. Oxford University Press, New York, p 480

Guibal D, Remacre AZ (1984) Local estimation of the recoverable reserves: comparing various methods with the reality on a porphyry copper deposit. In: Verly G, David M, Journel AG, Maréchal A (eds) Geostatistics for natural resources characterization. Reidel, Dordrecht, pp 435–448

Herzfeld UC (1989) A note on programs performing kriging with nonnegative weights. Math Geol 21(3):391–393

Hochstrasser UW (1972) Orthogonal polynomials. In: Abramowitz M, Stegun IA (eds) Handbook of mathematical functions. Dover Publications, New York, pp 771–802

Journel AG (1980) The lognormal approach to predicting local distributions of selective mining unit grades. Math Geol 12(4):285–303

Journel AG (1983) Non parametric estimation of spatial distributions. Math Geol 15(3):445–468

Journel AG, Huijbregts CJ (1978) Mining Geostatistics. Academic Press, London, p 600

Koziol JA (1986) Assessing multivariate normality: a compendium. Commun Stat Theory Methods 15:2763–2783

Maréchal A (1984) Recovery estimation: a review of models and methods. In: Verly G, David M, Journel AG, Maréchal A (eds) Geostatistics for natural resources characterization. Reidel, Dordrecht, pp 385–420

Matheron G (1971) The theory of regionalized variables and its applications. Ecole Nationale Supérieure des Mines de Paris, Fontainebleau, p 212

Matheron G (1974) Effet proportionnel et lognormalité ou: le retour du serpent de mer. Internal report N-374, Centre de Géostatistique, Ecole Nationale Supérieure des Mines de Paris, Fontainebleau, p 43

Matheron G (1976) A simple substitute for conditional expectation: the disjunctive kriging. In: Guarascio M, David M, Huijbregts CJ (eds) Advanced geostatistics in the mining industry. Reidel, Dordrecht, pp 221–236

Mecklin CJ, Mundfrom DJ (2004) An appraisal and bibliography of tests for multivariate normality. Int Stat Rev 72(1):123–138

Ortega J, Rheinboldt W (1970) Iterative solution of nonlinear equations in several variables. Academic Press (Computer Science and Applied Mathematics), New York, p 572

Parker HM, Journel AG, Dixon WC (1979) The use of conditional lognormal probability distribution for the estimation of open-pit ore reserves in stratabound uranium deposits—a case study. In: O'Neil TJ (ed) Proceedings of the 16th APCOM international symposium. Society of Mining Engineers of the AIME, New York, pp 133–148

Remacre AZ (1984) L'estimation du récupérable local – le conditionnement uniforme. Doctoral Thesis, Ecole Nationale Supérieure des Mines de Paris, Fontainebleau, p 99

Rendu JM (1979) Normal and lognormal estimation. Math Geol 11(4):407–422

Rivoirard J (1990) A review of lognormal estimators for in situ reserves. Math Geol 22(2):213–221

Rivoirard J (1994) Introduction to disjunctive kriging and nonlinear geostatistics. Oxford University Press, Oxford, p 181

Verly G (1983) The multigaussian approach and its applications to the estimation of local reserves. Math Geol 15(2):259–286

Verly G (1984) The block distribution given a point multivariate normal distribution. In: Verly G, David M, Journel AG, Maréchal A (eds) Geostatistics for natural resources characterization. Reidel, Dordrecht, pp 495–515