Mathematical Geology, Vol. 34, No. 1, January 2002 (© 2002)

Conditional Simulation of Nongaussian Random Functions[1]

Xavier Emery[2]

This paper presents a conditional simulation procedure that overcomes the limits of gaussian models and enables one to simulate regionalized variables with highly asymmetrical histograms or with partial or total connectivity of extreme values. The philosophy of the method is similar to that of sequential indicator technique, but it is more accurate because it is based on a complete bivariate model by means of an isofactorial law. The resulting simulations, which can be continuous or categorical, not only honor measured values at data points, but also reproduce the mono and bivariate laws of the random function associated to the regionalized variable, that is, every one or two-point statistic: histogram, variogram, indicator variograms. The "sequential isofactorial" method can also be adapted to conditional simulation of block values, without resorting to point–support simulations.

KEY WORDS: sequential indicator simulation, isofactorial models, disjunctive kriging, bivariate distribution.

INTRODUCTION

Geostatistical simulation techniques construct regionalized variables which show the same features as the one under study, noted $z(\mathbf{x})$ hereafter. Such a construction is based on the interpretation of $z(\mathbf{x})$ as *one* realization, or outcome, of a random function $Z(\mathbf{x})$, and consists in generating *other* realizations that constitute possible and equiprobable images of the reality (Journel and Huijbregts, 1978). For practical applications, conditional simulations are built, which honor measured values at sampling sites and reproduce the structural patterns of $z(\mathbf{x})$.

Each simulation can be manipulated as if it were the real regionalized variable and be processed through a nonlinear operator. Consequently, any quantity, not only the regionalized variable itself, can be evaluated thanks to a set of conditional simulations (many simulations are necessary to obtain a sensible average value and

[1]Received 2 June 2000; accepted 11 January 2001.

[2]Department of Mining Engineering, University of Chile, Avenida Tupper 2069, Santiago, Chile; e-mail: xemery@cec.uchile.cl

0882-8121/02/0100-0079/1 © 2002 International Association for Mathematical Geology

a range of possible situations). For example, in the mining field, the probability that the grade of a given block exceeds a cutoff can be estimated by the empirical frequency of simulated block values over such a cutoff. Another application of simulations is the assessment of the uncertainty attached to the quantity being studied, for example, via confidence intervals.

Countless geostatistical simulation techniques have been developed. Most of them rely on the gaussian probability law: decomposition of the covariance matrix, sequential gaussian simulation, turning bands, and spectral methods, to name a few (Alabert, 1987; Davis, 1987; Deutsch and Journel, 1998; Lantuéjoul, 1993; Matheron, 1973a). In the general case, the studied variable $Z(\mathbf{x})$ has to be transformed into a gaussian one $Y(\mathbf{x})$; such a transformation is referred to as "gaussian anamorphosis" or "normal score transform." At the end of the procedure, the inverse anamorphosis is applied to go back to the initial variable (Journel and Huijbregts, 1978). Using the gaussian probability law is very convenient, because it depends on few parameters (actually, it is enough to specify a single covariance function, because the gaussian transformed variable has a zero mean). However, several limitations restrict the generality of gaussian techniques:

- the gaussian anamorphosis may be arduous, especially when the regionalized variable under study has a highly skewed histogram or presents a high proportion of zero values or "ties" (Rivoirard, 1994);
- realizations of gaussian processes exhibit a symmetry with respect to the median value: the spatial patterns concerning low values also arise for high values;
- the occurrence of extreme values is purely random (this is known in mining geostatistics as the *destructuration of high grades* property). Gaussian models cannot describe phenomena where extreme values are spatially connected (Goovaerts, 1997; Matheron, 1982).

When gaussian simulation techniques are unsatisfactory, it is necessary to resort to either postprocessing algorithms in order to improve the obtained realizations, or nongaussian simulation methods, which allow for instance a clustering of extreme values. The problem of the latter is that they are time-consuming and approximate: in general, they are limited to the reproduction of part of the mono and bivariate laws (e.g., the histogram and covariance of the variable and/or some of its indicators) instead of the entire spatial law. The most widely used nongaussian algorithm is sequential indicator method (Alabert, 1987; Deutsch and Journel, 1998; Goovaerts, 1997; Journel, 1989), which is summarized in next section. Other simulation techniques are available when dealing with random sets and categorical variables: truncated plurigaussian method (Le Loc'h and others, 1994), and object-based algorithms like the Boolean models and their extensions (Chilès and Delfiner, 1999; Lantuéjoul, 1997).

THE SEQUENTIAL INDICATOR SIMULATION METHOD

This method is an iterative procedure, where each target point is successively simulated, taking into account the initial data values and the previously simulated values. More precisely, for each point being simulated, an estimation of its local cumulative density function is built, conditioned to both initial data values and already simulated values. This construction is achieved by way of an indicator kriging followed by a postprocessing step. The simulated value is drawn at random from the probability law corresponding to its local cumulative density function; for instance, it can be obtained from a uniformly distributed value in [0,1] by the inversion method.

Remarks

1. The sequential indicator method provides conditional simulations, which honor measured values at data sites, up to the resolution given by the indicator coding.
2. In theory, the sequential paradigm requires estimating each local cumulative density function from *all* the already simulated values. In practice, only those located in a neighborhood of the target site are retained. Hence, spatial variability is not reproduced perfectly, especially for long distances. Some procedures have been proposed to correct this problem; for instance, when simulating the nodes of a regular grid, the simulation can be achieved on a coarse grid first, and then be refined (concept of *multiple grid*) (Deutsch and Journel, 1998; Goovaerts, 1997).
3. In order to avoid artifacts in the final simulation, it is advisable to simulate the target sites in a random sequence.
4. The reproduction quality of the histogram of $Z(\mathbf{x})$ depends on the discretization level (number of indicators) and on the choice of the postprocessing procedure that follows indicator kriging. Typically, about 10 indicators are selected, for example, the deciles of the distribution of $Z(\mathbf{x})$. As regards the bivariate law, the algorithm does not ensure the reproduction of the covariance function of $Z(\mathbf{x})$; only the covariances of the indicators used to determine the local cumulative density functions are honored approximately.

The main advantage of the sequential indicator method is its flexibility, because it does not rely on the gaussian assumption. The features of the regionalized variable are not described by a single covariance function any more, but by the covariances of indicators associated to several thresholds; as a consequence, it may take a spatial correlation of extreme values into account. The indicator formalism also facilitates the coding of measurement uncertainty and secondary information.

As a counterpart, the implementation requires a major effort for inference and structural analysis (additionally, it is difficult to build a theoretically coherent set of indicator variogram models, because these variograms are not independent and cannot be chosen among all types of models). Furthermore, the sequential indicator algorithm is time-consuming, as each simulated site requires the kriging of several indicators, and approximate, due to several factors: the discretization in indicators, the limitation of the kriging neighborhood, the separate kriging of each indicator and its postprocessing. A method which aims to improve the reproduction of the bivariate law of the regionalized variable is presented in the following section.

SEQUENTIAL ISOFACTORIAL SIMULATION

It is possible to model the entire bivariate law when it is isofactorial, that is, when there exists a complete family of factors spatially uncorrelated. Some well-known examples are the bigaussian, bigamma, hermitian, Laguerre-type, and beta laws, as well as discrete laws such as the binomial, negative binomial, and Poisson (Chilès and Delfiner, 1999; Matheron, 1973b, 1975, 1976, 1984). The general form of an isofactorial bivariate probability density function between two values $Y(\mathbf{x}_1)$ and $Y(\mathbf{x}_2)$ is

$$f(y_1, y_2) = f(y_1) f(y_2) \sum_{p \geq 0} T_p \, \chi_p(y_1) \, \chi_p(y_2)$$

where $f(y)$ represents the marginal probability density of $Y(\mathbf{x})$; $(T_p)_p$ is a series of real coefficients whose values are contained in the interval $[-1; 1]$; and $(\chi_p)_p$ are the factors of the isofactorial law ($\chi_0 \equiv 1$).

T_p—one should actually write $T_p(\mathbf{x}_1, \mathbf{x}_2)$—is the correlation coefficient between $\chi_p[Y(\mathbf{x}_1)]$ and $\chi_p[Y(\mathbf{x}_2)]$. When considered as a function of $\mathbf{x}_1$ and $\mathbf{x}_2$, or more simply of $\mathbf{x}_2 - \mathbf{x}_1$, T_p turns out to be the correlogram of the factor of order p. It can be deduced from T_1, which, in most cases, is nothing but the correlogram of $Y(\mathbf{x})$ (the relationship between T_1 and T_p depends on the chosen isofactorial law). In brief, the structural analysis of $Y(\mathbf{x})$ is enough to specify the correlograms of all the factors of the bivariate law. Using a single correlogram is not a severe limitation, because other structural patterns of the regionalization are described by simple scalar parameters, according to the selected model.

In practice, a transformation—or anamorphosis—of the raw variable $Z(\mathbf{x})$ is necessary to turn it into a variable $Y(\mathbf{x})$ which follows an isofactorial law. Under this assumption, any function $\varphi[Y(\mathbf{x})]$ can be estimated by disjunctive kriging (Matheron, 1973b, 1976; Rivoirard, 1994). It requires expanding $\varphi[Y(\mathbf{x})]$ in a series of factors

$$\varphi\,[Y(\mathbf{x})] = \sum_{p \geq 0} \varphi_p \, \chi_p[Y(\mathbf{x})]$$

and estimating separately each factor by simple kriging

$$\{\varphi[Y(\mathbf{x})]\}^{\mathrm{DK}} = \sum_{p\geq 0} \varphi_p \{\chi_p[Y(\mathbf{x})]\}^{\mathrm{SK}}$$

In many cases, disjunctive kriging only requires estimating the first factors (to fix ideas, about 10), because the high degree factor covariances often tend to a nugget effect, so that the simple kriging of these factors becomes equal to their mean, which is 0. However, this property does not hold any more in some particular cases with a strong connectivity of high values (mosaic model for instance); the way in which convergence problems can be dropped in practical calculations will be seen later.

When a discretization of the $Y(\mathbf{x})$ values is considered, disjunctive kriging amounts to a full indicator simple cokriging (Rivoirard, 1994) and provides theoretically more accurate results than indicator kriging or its variants.

The φ_p coefficients are obtained from the relationship

$$\varphi_p = \int \varphi(y)\chi_p(y) f(y)\, dy$$

Now, the disjunctive kriging estimator can be written as

$$\begin{aligned}\{\varphi[Y(\mathbf{x})]\}^{\mathrm{DK}} &= \int \varphi(y) f(y) \sum_{p\geq 0} \chi_p(y)\{\chi_p[Y(\mathbf{x})]\}^{\mathrm{SK}}\, dy \\ &= \int \varphi(y) f_{\mathrm{DK}}(\mathbf{x}; y \mid (n))\, dy \qquad (1)\end{aligned}$$

$$\text{with} \quad f_{\mathrm{DK}}(\mathbf{x}; y \mid (n)) = f(y) \sum_{p\geq 0} \chi_p(y)\{\chi_p[Y(\mathbf{x})]\}^{\mathrm{SK}}$$

(the symbol (n) refers to the n data used in the simple kriging).

This formula is comparable with the one of the conditional expectation of $\varphi[Y(\mathbf{x})]$

$$\{\varphi[Y(\mathbf{x})]\}^{\mathrm{CE}} = \int \varphi(y) f(\mathbf{x}; y \mid (n))\, dy$$

where $f(\mathbf{x}; y \mid (n))$ stands for the conditional probability density.

By analogy, the function $f_{\mathrm{DK}}(\mathbf{x}; y \mid (n))$ in Equation (1) has the meaning of a conditional probability density. It is called *pseudo density of disjunctive kriging*

(Matheron, 1976). It can be associated to a pseudo cumulative density function

$$F_{\mathrm{DK}}(\mathbf{x}; y \mid (n)) = \sum_{p \geq 0} \{\chi_p[Y(\mathbf{x})]\}^{\mathrm{SK}} \int_{-\infty}^{y} f(u)\chi_p(u)\, du \tag{2}$$

which is a "pseudo probability" that the value of $Y(\mathbf{x})$ is less than the y threshold, conditionally to the data values used in the simple kriging systems. As the first factor, χ_0, is equal to 1, Equation (2) can also be written as

$$F_{\mathrm{DK}}(\mathbf{x}; y \mid (n)) = F(y) + \sum_{p \geq 1} \{\chi_p[Y(\mathbf{x})]\}^{\mathrm{SK}} \int_{-\infty}^{y} f(u)\chi_p(u)\, du \tag{3}$$

F_{DK} appears as the prior cumulative density function $F(y)$, corrected by a series of terms that reflect the intensity of conditioning; these terms will be small in zones where data are scarce.

The integrals can be expressed analytically by means of the factors and can be calculated exactly. Although F_{DK} is equal to 0 in $-\infty$ and to 1 in $+\infty$, it may not be a cumulative density function, because it is not necessarily monotonous. However, it can be postprocessed into a "real" cumulative density function, conditioned by the data used in the simple kriging of the factors.

This statement enables one to build a sequential simulation algorithm identical to the sequential indicator one, except it uses F_{DK} as the local cumulative density function instead of estimating it by indicator kriging. The application of such a procedure directly gives conditional simulations, which reproduce the monovariate law (histogram) and the bivariate law (variogram, indicator variograms . . .) of the regionalized variable. As in the sequential indicator algorithm, it is advisable to simulate the target sites in a random sequence, and restrict the conditioning data (initial data and already simulated values) to those contained in a neighborhood of the site being simulated.

Remarks

1. Like the sequential indicator method, this technique has great flexibility: the various isofactorial models can describe satisfactorily most practical situations. For instance, in the Laguerre-type model, which uses the gamma law instead of the gaussian law, some parameters help to control the skewness of the distribution and the connectivity of the extreme values. Such structural patterns can therefore be reflected in the simulations.
2. With respect to the sequential indicator method, the computation time is similar (it requires the kriging of several factors, instead of the kriging of several indicators). However, the isofactorial procedure is more precise,

because it is based on the *complete* bivariate law, and determines the entire local cumulative density function, avoiding the discretization into indicators.[3] Moreover, it requires less inference effort, as shown further in the application, and the use of an isofactorial law ensures the coherence of the model (coherence between the indicator covariances).

3. When extreme values are highly correlated, convergence problems in the factorial expansions may occur. The velocity with which the factor covariances converge to a nugget effect may be very slow, so that a simple truncation of the expansions to a limited number of factors can result problematic. In practice, in such a case, observation shows that the kriging weights vary when estimating the first factors χ_p, $p = 1, \ldots, P_{\max} - 1$, and then become stable (usually, $P_{\max} \leq 15$). For the practical evaluation of the local cumulative density function, the following fairly accurate formula avoids convergence problems

$$F_{\mathrm{DK}}(\mathbf{x}; y \mid (n)) \approx F(y)\left[1 - \sum_{\alpha} \lambda_{\alpha}^{P_{\max}}\right] + \sum_{\alpha} \lambda_{\alpha}^{P_{\max}} I(\mathbf{x}_{\alpha}; y) + \sum_{p=1}^{P_{\max}-1} \sum_{\alpha} \left(\lambda_{\alpha}^{p} - \lambda_{\alpha}^{P_{\max}}\right) \chi_p[Y(\mathbf{x}_{\alpha})] \int_{-\infty}^{y} f(u)\chi_p(u)\, du \tag{4}$$

where $\{\mathbf{x}_{\alpha}, \alpha = 1, \ldots, n\}$ stand for the data points; $I(\mathbf{x}_{\alpha}; y)$ is the indicator associated to the y threshold in site $\mathbf{x}_{\alpha}$

$$I(\mathbf{x}_{\alpha}; y) = 1 \quad \text{if} \quad Y(\mathbf{x}_{\alpha}) < y, \quad 0 \text{ otherwise}$$

λ_{α}^{p} are the simple kriging weights for the factor χ_p

$$\{\chi_p[Y(\mathbf{x})]\}^{\mathrm{SK}} = \sum_{\alpha} \lambda_{\alpha}^{p}\, \chi_p[Y(\mathbf{x}_{\alpha})]$$

Equation (4) has the advantage of being exact in both limiting cases:

(a) in case of a total destructuration of extreme values, the factor covariances tend to a pure nugget effect, and the kriging weights λ_{α}^{p} quickly converge to 0 as p increases, so that Equation (3) truncated at order

[3]Considering the definition of disjunctive kriging as an indicator cokriging, it can be said that the sequential isofactorial method uses an infinite number of indicators, and determines the local cumulative density function by a *full* indicator cokriging, instead of a separate kriging.

$p = P_{\max}$ is met

$$F_{\mathrm{DK}}(\mathbf{x}; y \mid (n)) = F(y) + \sum_{p=1}^{P_{\max}-1} \{\chi_p[Y(\mathbf{x})]\}^{\mathrm{SK}} \times \int_{-\infty}^{y} f(u)\chi_p(u)\,du \tag{5}$$

(b) in case of a total structuration, the factors have the same covariance function and the kriging weights do not change with the order p; in this case, $F_{\mathrm{DK}}(\mathbf{x}; y \mid (n))$ is obtained by simple kriging of the indicator associated to the y threshold

$$F_{\mathrm{DK}}(\mathbf{x}; y \mid (n)) = I(\mathbf{x}; y)^{\mathrm{SK}} = F(y)\left[1 - \sum_{\alpha} \lambda_{\alpha}^{1}\right] + \sum_{\alpha} \lambda_{\alpha}^{1}\, I(\mathbf{x}_{\alpha}; y) \tag{6}$$

The idea for obtaining of Equation (4) originates from Rivoirard (1994) when dealing with stationarity problems in disjunctive kriging. It comes from Equation (3) and can be written as

$$F_{\mathrm{DK}}(\mathbf{x}; y \mid (n)) = F(y) + \sum_{p\geq 1} \sum_{\alpha} \lambda_{\alpha}^{p}\, \chi_p[Y(\mathbf{x}_{\alpha})] \int_{-\infty}^{y} f(u)\chi_p(u)\,du$$

Splitting the series into a partial sum until order $P_{\max} - 1$ and a sum from order $P_{\max}$ to infinite, and considering that, for $p \geq P_{\max}$, the correlogram T_p varies very slowly with respect to p (empirical observation), so that the kriging weights are almost equal to those of order $P_{\max}$, one obtains

$$\begin{aligned} F_{\mathrm{DK}}(\mathbf{x}; y \mid (n)) &\approx F(y) + \sum_{p=1}^{P_{\max}-1} \sum_{\alpha} \lambda_{\alpha}^{p}\, \chi_p[Y(\mathbf{x}_{\alpha})] \int_{-\infty}^{y} f(u)\chi_p(u)\,du \\ &\quad + \sum_{\alpha} \lambda_{\alpha}^{P_{\max}} \sum_{p\geq P_{\max}} \chi_p[Y(\mathbf{x}_{\alpha})] \int_{-\infty}^{y} f(u)\chi_p(u)\,du \\ &\approx F(y)\left[1 - \sum_{\alpha} \lambda_{\alpha}^{P_{\max}}\right] + \sum_{p=1}^{P_{\max}-1} \sum_{\alpha} \left(\lambda_{\alpha}^{p} - \lambda_{\alpha}^{P_{\max}}\right) \\ &\quad \times \chi_p[Y(\mathbf{x}_{\alpha})] \int_{-\infty}^{y} f(u)\chi_p(u)\,du \\ &\quad + \sum_{\alpha} \lambda_{\alpha}^{P_{\max}} \sum_{p\geq 0} \chi_p[Y(\mathbf{x}_{\alpha})] \int_{-\infty}^{y} f(u)\chi_p(u)\,du \end{aligned}$$

Now, for a data point $\mathbf{x}_\alpha$, the (pseudo) cumulative density function is a step function. Hence

$$F_{\mathrm{DK}}(\mathbf{x}_\alpha; y \mid (n)) = \sum_{p \geq 0} \chi_p[Y(\mathbf{x}_\alpha)] \times \int_{-\infty}^{y} f(u)\chi_p(u)\, du = I(\mathbf{x}_\alpha; y)$$

which completes the explanation for using Equation (4).

4. The sequential isofactorial method enables one to simulate block values without resorting to point–support simulations, thanks to the so-called discrete isofactorial models. These models assume that the point and block distributions follow, after anamorphosis, isofactorial laws, and that the distribution between points and blocks follows an asymmetrical isofactorial law. Such a law is defined by two families of factors: $\chi_p^{(1)}$ and $\chi_p^{(2)}$, respectively associated to the points and the blocks; as an operating rule, two factors are spatially uncorrelated when they have different degrees. It is then possible to determine all the correlation functions between point and block values, which allows the estimation of the block factors by cokriging from known point and block values. The conditional cumulative density function of a block v is derived as

$$F_{\mathrm{DK}}(v; y \mid (n)) = F_v(y) + \sum_{p \geq 1} \left\{\chi_p^{(2)}(Y_v)\right\}^{\mathrm{SCK}} \int_{-\infty}^{y} f_v(u)\chi_p^{(2)}(u)\, du \quad (7)$$

where Y_v stands for the transformed value of block v (i.e., after anamorphosis); f_v and F_v are the standard and cumulative prior density functions of Y_v; and the SCK index refers to simple cokriging from initial point–support values and already simulated block values.

This approach—direct conditional simulation of block values—is *not* possible with the sequential indicator algorithm, unless strong and awkward approximations are made (e.g., affine correction to obtain a block local cumulative density function from a point–support one). It can be achieved in a gaussian context, via any simulation algorithm, using the discrete gaussian model (Rivoirard, 1994), which actually belongs to the family of isofactorial models.

5. The drawbacks of the sequential isofactorial procedure are similar to those of the sequential indicator method: the computation time is high—though acceptable—and some approximations are indispensable: restriction of the kriging neighborhood and postprocessing of the pseudo local cumulative density functions.

A Word on Stationarity

Particular attention should be paid to the assumption of stationarity. As it has been presented, the isofactorial method requires the regionalized variable under study to be a realization of a stationary process, because it makes use of a simple kriging with zero mean. Such an assumption is a rather demanding prerequisite and the question of weakening it should be examined.

On the one hand, there is no convenient way of checking the stationarity of a regionalized variable: it is a theoretical notion and may be acceptable despite the appearance (refer for instance to the "proportional effect" property which occurs with lognormally distributed variables and is compatible with the assumption of strict stationarity). On the other hand, it is possible, in point–support simulations only, to use an ordinary kriging of the factors instead of a simple kriging, although this approach leads to theoretical difficulties (Rivoirard, 1994). A research topic could deal with the capability of transferring the possible nonstationarity into the anamorphosis function instead of the transformed variable.

EXAMPLES

To illustrate what has been said, Figure 1 displays six bidimensional realizations of isofactorial models, represented in gray-scale maps:

(a) *Bigaussian model* (Fig. 1(A)). It is a restriction of the multigaussian model and has the same limitations (symmetry with respect to the median value, spatial uncorrelation of extreme values); the factors are the normalized Hermite polynomials (Matheron, 1973b, 1976; Rivoirard, 1994)

$$\chi_p(y) = \frac{1}{\sqrt{p!}\, e^{-y^2/2}} \frac{d^p}{dy^p} \left(e^{-y^2/2}\right), \quad \text{with } p \in \mathbb{N}$$

(b) *Hermitian model* (Fig. 1(B)). It generalizes the bigaussian model, because it considers an additional coefficient which measures the destructuration of high values (Chilès and Delfiner, 1999; Matheron, 1975, 1976). This destructuration coefficient can be specified by comparing the variogram of the gaussian variable with its madogram (first order variogram).

(c) *Bigamma model* (Fig. 1(C)). It is based on the gamma law, which depends on a parameter ruling its asymmetry. It can describe regionalized variables with a highly skewed distribution, for which the gaussian transformation fails (Hu, 1988; Matheron, 1973b, 1984). The factors associated to the

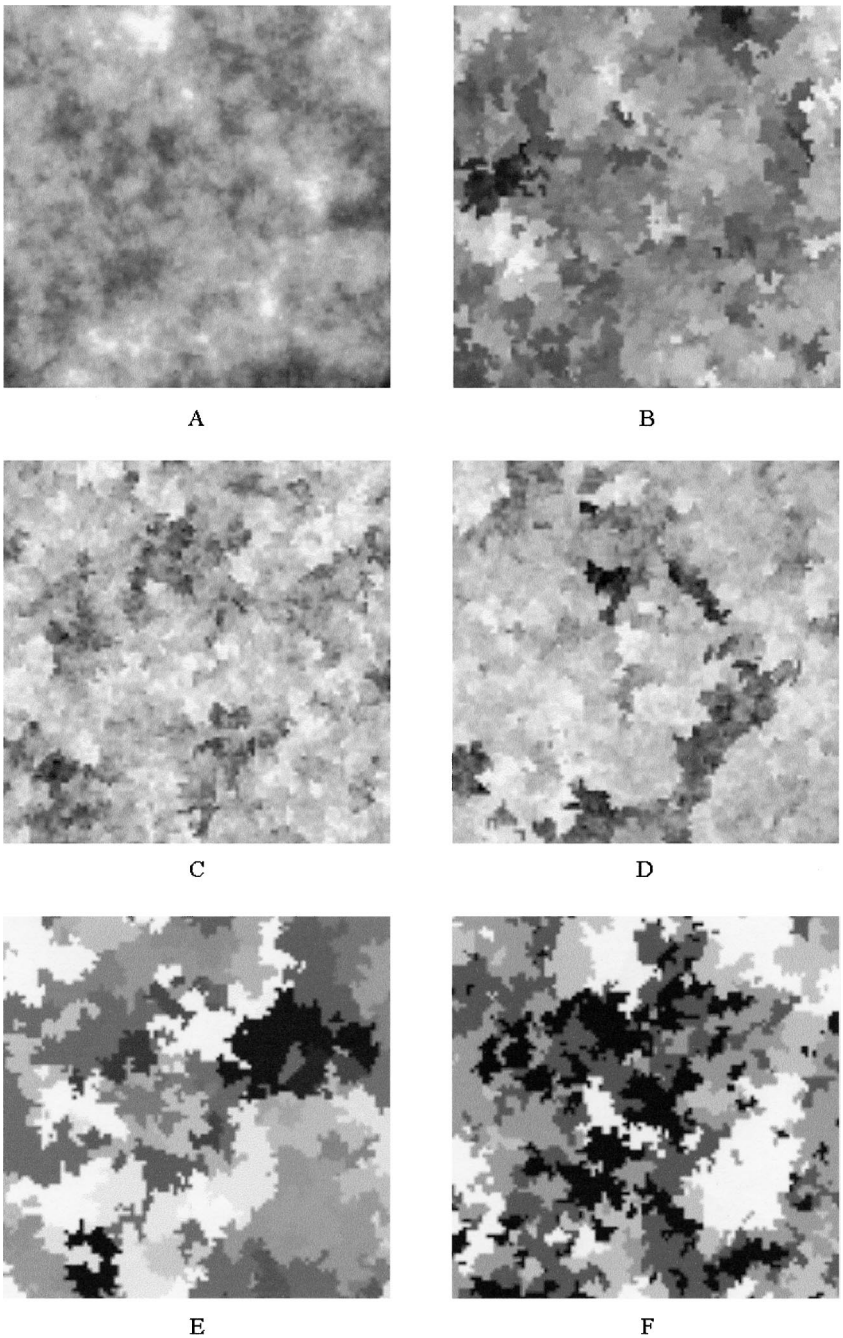

Figure 1. Realizations of (A) bigaussian, (B) hermitian, (C) bigamma, (D) Laguerre-type, (E) mosaic, and (F) orthogonal indicator residuals processes.

bigamma law of parameter α are the normalized Laguerre polynomials of order α

$$\chi_p(y) = \sqrt{\frac{\Gamma(\alpha)}{p!\Gamma(\alpha+p)}}\ \frac{1}{e^{-y}y^{\alpha-1}}\ \frac{d^p}{dy^p}(e^{-y}\,y^{p+\alpha-1}), \quad \text{with } p \in \mathbb{N}$$

(d) *Laguerre-type model* (Fig. 1(D)). It generalizes the bigamma model by adding a coefficient which controls the destructuration of extreme values (Chilès and Delfiner, 1999; Matheron, 1975); Figure 1(D) considers a positively skewed distribution as well as a partial connectivity of high values.

(e) *Mosaic model* (Fig. 1(E)). Actually, it is a particular case of the hermitian and Laguerre-type models, where there is no destructuration of extreme values, as opposed to the bigaussian or bigamma models, where the destructuration is total (Matheron, 1982); the image appears as more "ordered."

(f) *Orthogonal indicator residuals model* (Fig. 1(F)). This model describes categorical variables without edge effects when going upwards or downwards (Rivoirard, 1989); only the mosaic model combines the absence of edge effects in both senses.

No initial data are considered in the simulations, which are *not* conditional. The realizations share the same covariance (an exponential model); however, their bivariate laws are different. They illustrate the flexibility of the sequential isofactorial method, which can reproduce a great variety of structural characteristics.

APPLICATION TO A MINING DATASET

In this section, the sequential isofactorial method is applied to a dataset from a gold deposit. It deals with 3810 composite samples of 5 m length (Fig. 2), with their gold grade (unit: g/t). Because of the irregular sampling, a declustering variable is taken into account in the calculation of the data histogram and the associated statistics (Fig. 3). This variable is determined by the cell method (Deutsch and Journel, 1998), with a reference cell of size 40 m $\times$ 40 m $\times$ 5 m; these dimensions correspond approximately to the mean separation between samples.

The histogram shows a strong asymmetry as well as "ties" in its origin, which would make approximate any attempt of gaussian anamorphosis and clumsy the use of a gaussian model. To describe the gold grade, a Laguerre-type model is

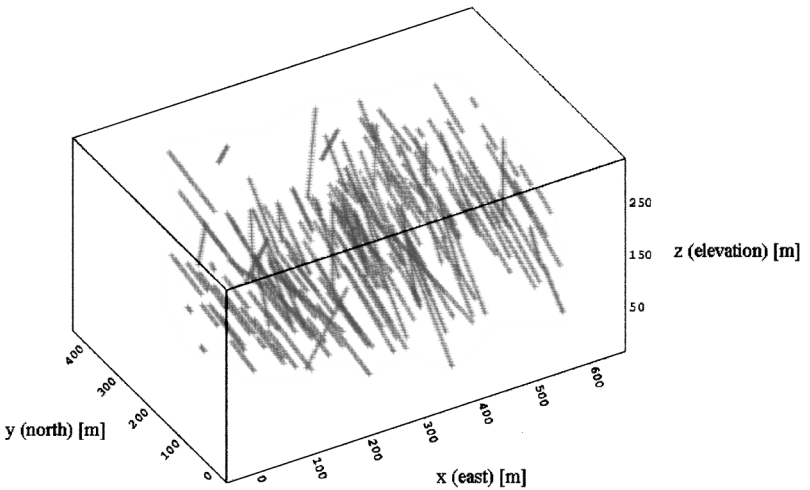

Figure 2. Base map of the samples (perspective view).

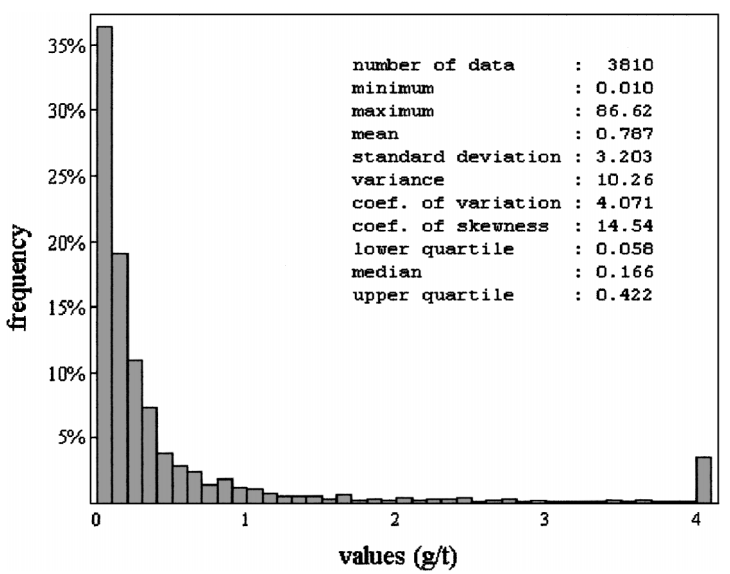

Figure 3. Declustered histogram of the gold data (restricted to the values between 0 and 4 g/t).

considered because it incorporates two specific parameters which will be quite pertinent in this study:

- a skewness coefficient, noted α;
- a destructuration coefficient, noted β.

Determination of the Point–Support Model

First, an anamorphosis is achieved in order to transform the initial variable $Z(\mathbf{x})$ into a variable $Y(\mathbf{x})$ which follows a gamma distribution (Fig. 4). Now, this distribution depends on a skewness coefficient, which controls its form. In this case, the value $\alpha = 0.5$ has been retained, because the corresponding anamorphosis leaves unchanged the ratio between the mean and the median; in addition, such a coefficient value is compatible with the presence of ties in the histogram origin, as it is less than 1. This and other criteria for choosing the skewness coefficient are presented in Hu (1988).

The empirical anamorphosis, which is a step function, is usually modeled via an expansion in a series of factors (Laguerre polynomials). The key parameter in this modeling is the choice of the limits of the raw variable, here [0,100 g/t].

The destructuration coefficient can be identified thanks to a plot of the experimental values of the first order variogram or "madogram," $\gamma_1(\mathbf{h})$, versus those of the second order variogram, $\gamma(\mathbf{h})$ (Fig. 5(A)); to improve the identification of such a coefficient, calculations along one direction of high continuity were superimposed to omnidirectional calculations.

In theory, these variograms are linked through the relation

$$\gamma_1(\mathbf{h}) = \frac{\Gamma(\alpha + 1/2)\Gamma(\beta)}{\sqrt{\pi}\Gamma(\alpha)\Gamma(\beta + 1/2)} \frac{\Gamma(\beta\gamma(\mathbf{h})/\alpha + 1/2)}{\Gamma(\beta\gamma(\mathbf{h})/\alpha)} \tag{8}$$

where Γ stands for the Euler function which interpolates the factorial.

The coefficient β has to be found so that Equation (8) is verified approximately by the experimental points in Figure 5(A). A coefficient equal to 0.4 leads to a satisfactory fitting (Fig. 5(B)).

The structural analysis of the gamma variable $Y(\mathbf{x})$ has to be performed to complete the point–support model. This variable shows an anisotropy whose minor range direction is oriented 30° from the vertical axis, whereas the orthogonal plane is quite isotropic. Such an anisotropy orientation is corroborated by geological information. The correlogram model (Fig. 6) contains a nugget effect and a spherical structure (the use of a correlogram is due to the lack of robustness of the classical variogram, because of the strong asymmetry of the gamma variable distribution and the presence of extreme values).

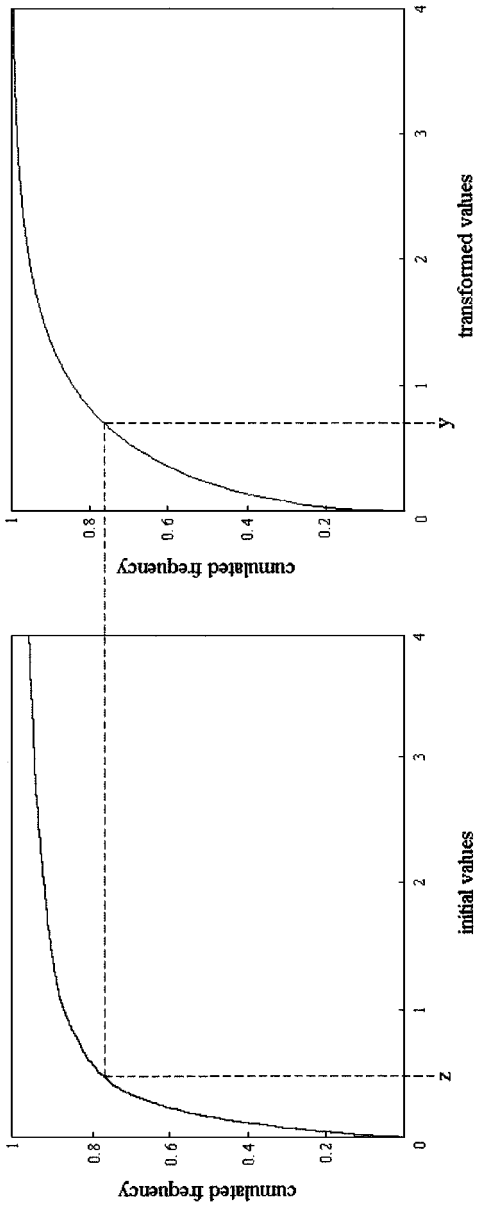

Figure 4. Graphical construction of the anamorphosis function. (A) Experimental cumulated declustered histogram; (B) Gamma cumulative density function with coefficient $\alpha = 0.5$.

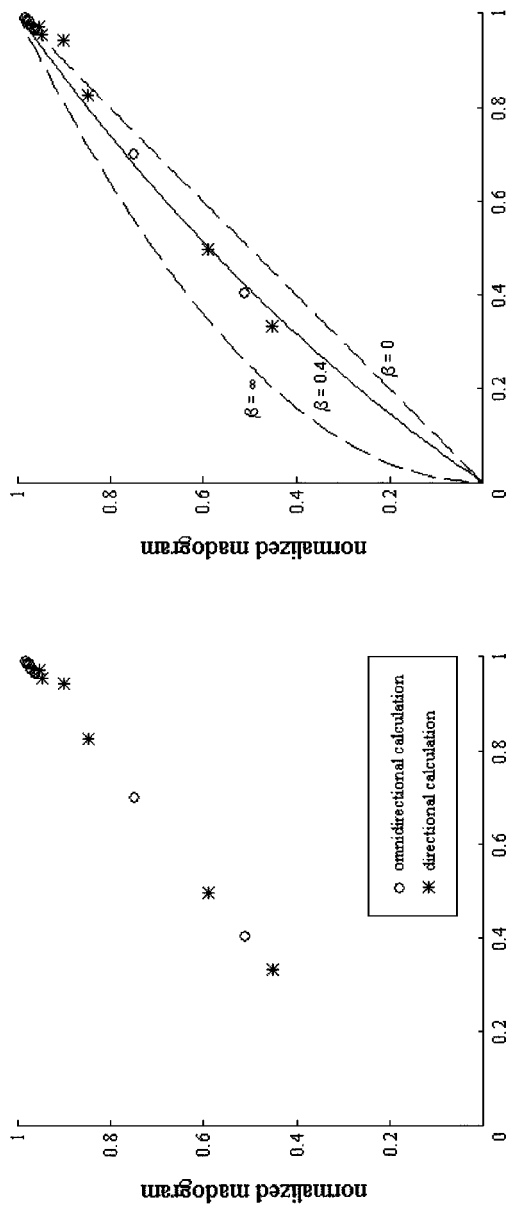

Figure 5. (A) First order normalized experimental variogram versus the second order one; (B) Fitting of the destructuration coefficient β (continuous line), dot lines: $\beta = 0$ (mosaic model) and $\beta = \infty$ (pure bigamma model).

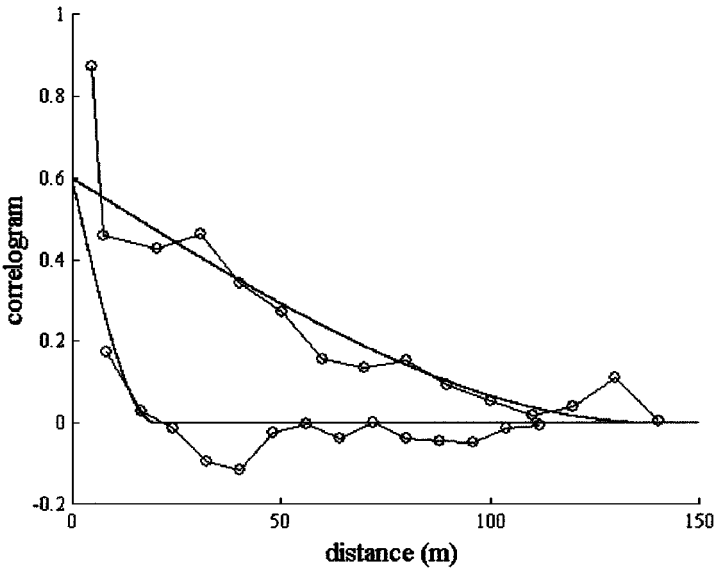

Figure 6. Experimental and modeled correlograms along the principal anisotropy directions.

Validation of the Isofactorial Property

The bivariate model can be validated by comparing several indicator variograms with their theoretical expressions, which can be deduced from the correlogram of $Y(\mathbf{x})$ and the coefficients α and β (Fig. (7)).

The conformity between experimental and theoretical curves is satisfactory: the bivariate model proves to be adequate. Note that, contrary to the bigaussian model, here the first and third quartile variograms (Fig. 7(A) and (C)) are not identical any more, although they correspond to symmetrical low and high quantiles; thus, the Laguerre-type model is able to take into account a greater correlation of high values than of low values.

Point–Support Simulations

As the point–support isofactorial model is entirely specified, various simulations can be made thanks to the sequential isofactorial method (Fig. 8). The images obtained have the same structural features as regards the anisotropy and the connectivity of high values. Conditioning to data values is also visible, as they globally show the same high grade and low grade areas.

The selective mining units correspond to blocks of size 4 m $\times$ 4 m $\times$ 5 m. To obtain simulations of block values, a first solution consists in averaging

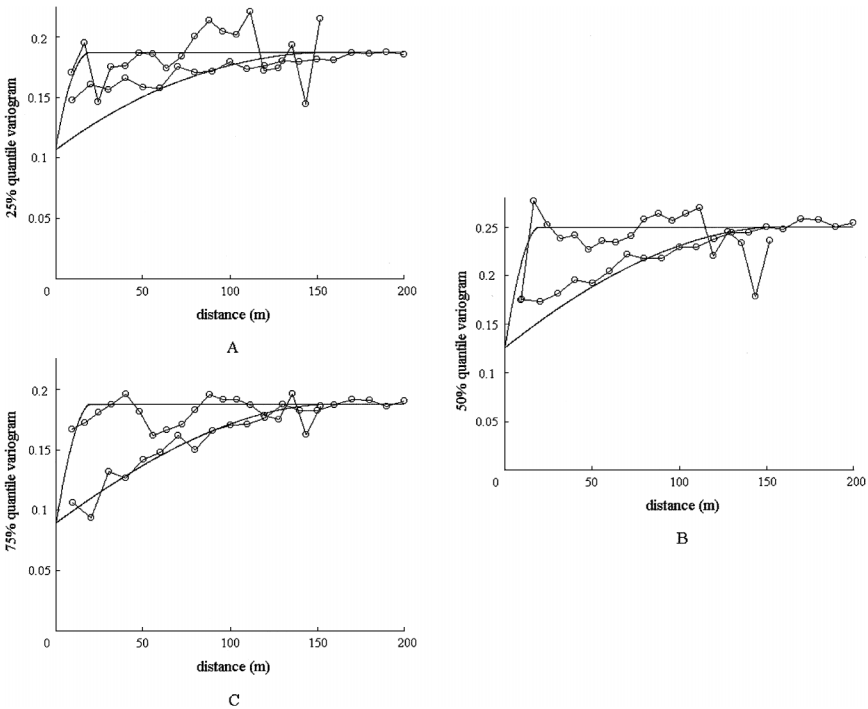

Figure 7. Experimental and theoretical variograms of the cumulated indicators associated to (A) the first quartile, (B) the median, and (C) the third quartile.

point–support simulations, which requires discretizing each block into several points. Hereafter, a variant of the method is described: it allows one to *directly* simulate block values, without using point–support simulations, which considerably alleviates the amount of calculations. As a counterpart, additional assumptions are needed in order to build a change of support model.

Block Simulations

The change of support model assumes that point and block values follow, after anamorphosis, isofactorial Laguerre-type laws, and that the law between points and blocks is isofactorial and asymmetrical. Such a law is characterized by two series of factors, which are Laguerre polynomials (Chilès and Delfiner, 1999). To ensure the coherence of the model, the positions of the samples must be randomized inside the blocks. The modus operandi is similar to the one used in the well-known *discrete gaussian model* (Rivoirard, 1994) and will not be detailed hereafter.

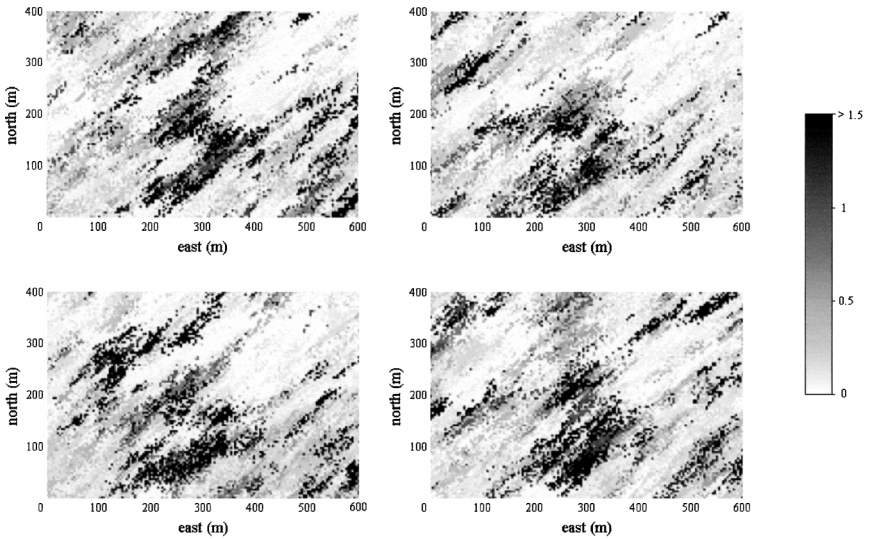

Figure 8. Four conditional simulations of the point–support gold grade (representation of a horizontal bench).

With respect to the point–support model, several additional parameters have to be specified:

- the change of support coefficient, which measures the correlation between a block value and the point–support values inside this block;
- the correlogram of block values after anamorphosis;
- the skewness coefficient of block values, which is partly undetermined.

Once known these parameters, all the covariance functions between point and block factors are fully determined; the block associated factors can then be estimated by simple cokriging from any set of point and block factor values. Using this cokriging in the sequential algorithm for calculating the block local cumulative density functions, enables one to build direct conditional simulations of block values (Fig. 9).

Block simulations can help to estimate the transfer functions associated to recoverable reserves (e.g., tonnage and metal quantity above a given cutoff). Though these functions can be evaluated analytically via disjunctive kriging, the advantage of the simulations is their flexibility. Firstly, they allow to chose the quality criterion for an estimation. For instance, each block can be classified into mineral or waste by minimizing a loss function which takes into account economical and practical parameters, whereas the estimations by disjunctive kriging are based on the minimization of the mean squared error. Secondly, unlike disjunctive kriging,

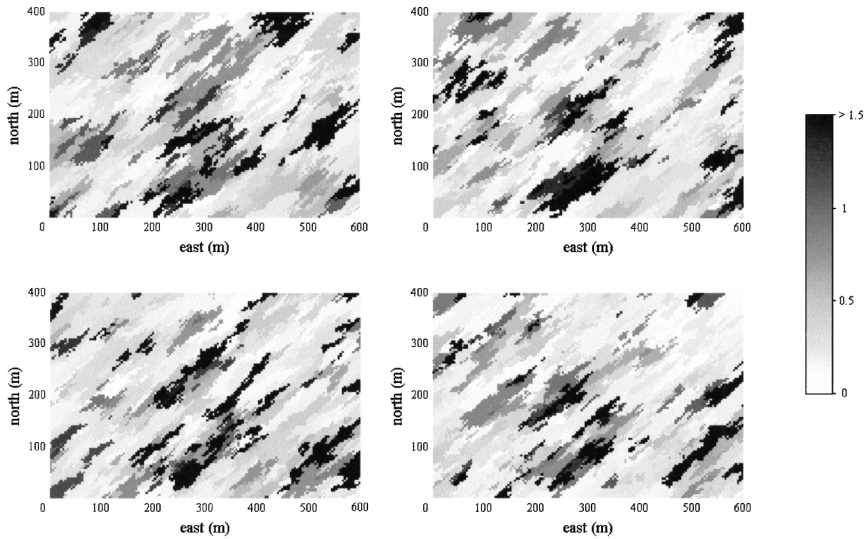

Figure 9. Four conditional simulations of the block–support gold grade (representation of a horizontal bench).

simulations can be used to study several blocks *simultaneously*, for example, the blocks of a same panel.

CONCLUSION

The sequential isofactorial method provides conditional simulations which reproduce the mono and bivariate distributions of the variable under study, improving the quality of algorithms based on an indicator discretization. It is quite a flexible technique, because it allows the user to regulate features that cannot be considered in the gaussian frame, namely the skewness of the distribution and/or the connectivity of high values; it can be adapted to the simulation of continuous or categorical variables, as well as direct simulation of block average values.

Like other sequential simulation techniques, some approximations are inevitable (restriction of the conditioning neighborhood, monotonicity correction of the local cumulative density function), but the quality of the algorithm remains excellent. As an example, Figure 10 compares the empirical and theoretical variograms and madograms (first order variograms) of the realizations corresponding to the hermitian and Laguerre-type processes shown in Figure 1(B) and (D); because these processes have the same theoretical normalized variogram (an exponential model) and the same destructuration coefficient, they also share the same normalized madogram according to Equation (8).

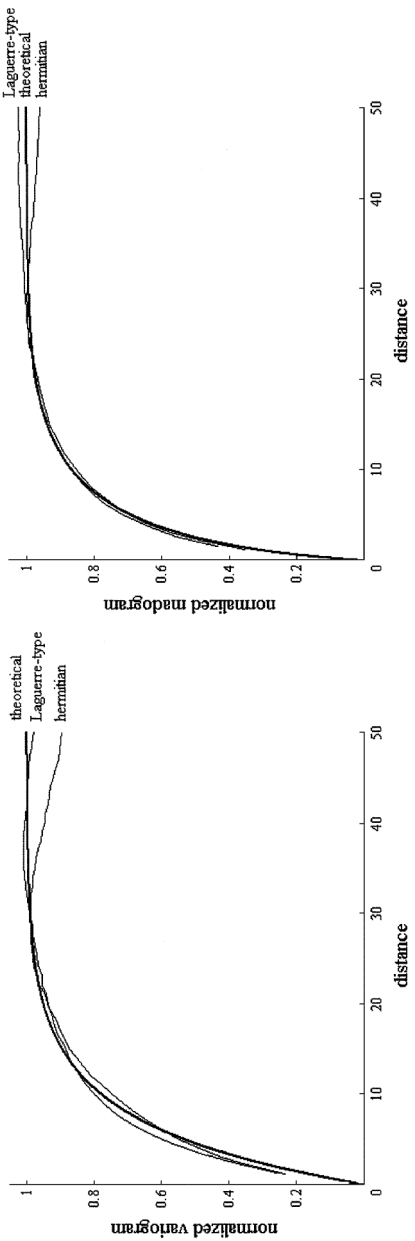

Figure 10. Theoretical and empirical normalized (A) variograms and (B) madograms for two realizations of Figure 1.

REFERENCES

Alabert, F., 1987, Stochastic imaging of spatial distributions using hard and soft information: Unpublished master's thesis, Department of Applied Earth Sciences, Stanford University, Stanford, California, 198 p.

Chilès, J. P., and Delfiner, P., 1999, Geostatistics: Modeling spatial uncertainty: Wiley, New York, 696 p.

Davis, M. W., 1987, Production of conditional simulations via the LU triangular decomposition of the covariance matrix: Math. Geology, v. 19, no. 2, p. 91–98.

Deutsch, C. V., and Journel, A. G., 1998, GSLIB: Geostatistical software library and user's guide, 2nd ed.: Oxford University Press, New York, 369 p.

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

Hu, L.-Y., 1988, Mise en œuvre du modèle gamma pour l'estimation des distributions spatiales: Unpublished doctoral dissertation, Centre de Géostatistique, Ecole Nationale Supérieure des Mines de Paris, Fontainebleau, 142 p.

Journel, A. G., 1989, Fundamentals of geostatistics in five lessons, Vol. 8: Short course in geology: American Geophysical Union, Washington, DC, 91 p.

Journel, A. G., and Huijbregts, Ch. J., 1978, Mining geostatistics: Academic Press, London, 600 p.

Lantuéjoul, C., 1993, Nonconditional simulation of stationary isotropic multigaussian random functions, *in* Armstrong, M., and Dowd, P. A., eds., Geostatistical simulations: Kluwer Academic, Dordrecht, Holland, p. 147–177.

Lantuéjoul, C., 1997, Iterative algorithms for conditional simulation, *in* Baafi, E. Y., and Schofield, N. A., eds., Geostatistics Wollongong'96: Kluwer Academic, Dordrecht, Holland, p. 27–40.

Le Loc'h, G., Beucher, H., Galli, A., Doligez, B., and Heresim Group., 1994, Improvement in the truncated Gaussian method: Combining several Gaussian functions, *in* Proc. ECMOR IV, Fourth European Conference on the Mathematics of Oil Recovery, Røros, Norway, 7–10 June 1994, Topic B: Heterogeneity Description and Assessment of Uncertainty, 13 p.

Matheron, G., 1973a, The intrinsic random functions and their applications: Advances in applied probability, Vol. 5, p. 439–468.

Matheron, G., 1973b, Le krigeage disjonctif: Internal report N-360, Centre de Géostatistique, Ecole Nationale Supérieure des Mines de Paris, Fontainebleau, 40 p.

Matheron, G., 1975, Compléments sur les modèles isofactoriels: Internal report N-449, Centre de Géostatistique, Ecole Nationale Supérieure des Mines de Paris, Fontainebleau, 21 p.

Matheron, G., 1976, A simple substitute for conditional expectation: The disjunctive kriging, *in* Guarascio, M., David, M., and Huijbregts, Ch. J., eds., Advanced geostatistics in the mining industry: NATO ASI Series C-24, Reidel, Dordrecht, Holland, p. 221–236.

Matheron, G., 1982, La déstructuration des hautes teneurs et le krigeage des indicatrices: Internal report N-761, Centre de Géostatistique, Ecole Nationale Supérieure des Mines de Paris, Fontainebleau, 33 p.

Matheron, G., 1984, Isofactorial models and change of support, *in* Verly, G., David, M., Journel, A. G., and Marechal, A., eds., Geostatistics for natural resources characterization: NATO ASI Series C-122, Reidel, Dordrecht, Holland, p. 449–467.

Rivoirard, J., 1989, Models with orthogonal indicator residuals, *in* Armstrong, M., ed., Geostatistics, Vol. 1: Kluwer Academic, Dordrecht, Holland, p. 91–108.

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