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Comparing sequential Gaussian and turning bands algorithms for cosimulating grades in multi-element deposits

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ABSTRACT

Stochastic simulation is increasingly used to map the spatial variability in the grades of elements of interest and to assess the uncertainty in the mineral resources and ore reserves. The practical implementation requires specifying a stochastic model, which describes the spatial distribution of the grades, and an algorithm to construct realizations of these grades, viewed as different possible outcomes or scenarios. In the case of the Gaussian random field model, a variety of algorithms have been proposed in the past decades, but their ability to reproduce the model statistics is often unequal. In this paper, we compare two such algorithms, namely the turning bands and the sequential algorithms. The comparison is hold through a synthetic case study and a real case study in a porphyry copper deposit located in southeastern Iran, in which it is of interest to jointly simulate the copper, molybdenum, silver, lead and zinc grades. Statistical testing and graphical validations are realized to check whether or not the realizations reproduce the features of the true grades, in particular their direct and cross variograms. Sequential simulation based on collocated cokriging turns out to poorly reproduce the cross variograms, while turning bands proves to be accurate in all the analyzed cases.

1. Introduction

Geostatistical simulation is widely used in the evaluation of mineral resources and ore reserves to map geological heterogeneity at different spatial scales and to assess the uncertainty in the unknown values of coregionalized variables, such as the grades of elements of interest, petrophysical properties of the subsoil, or geometallurgical properties (work index, acid consumption, metal recoveries) (Boisvert et al., 2013; Rossi and Deutsch, 2014). Its practical implementation requires specifying a stochastic model, which describes the spatial distribution of the coregionalized variables (*what* should be simulated), and an algorithm, which aims at constructing realizations of the prescribed model (*how* it should be simulated) (Chilès and Delfiner, 2012; Lantuéjoul, 2002).

When the coregionalized variables can be modeled (up to some nonlinear transformation) by Gaussian random fields, a few exact algorithms, such as the matrix decomposition (Davis, 1987, Myers, 1989), discrete spectral (Chilès and Delfiner, 1997; Dietrich and Newsam, 1993; Le Ravalec et al., 2000 Pardo-Igúzquiza and Chica-Olmo, 1993) and moving average (Black and Freyberg, 1990) algorithms, perfectly reproduce their joint distribution and spatial correlation structure, but such algorithms are limited, either because they cannot be used for large-scale problems or because they require the data and target locations to be regularly spaced.

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To overcome these limitations, approximate algorithms can be applied, allowing dealing with large numbers of data on unstructured grids. In this category, one finds the sequential Gaussian (Deutsch and Journel, 1998), continuous spectral (Shinozuka and Jan, 1972) and turning bands (Matheron, 1973) algorithms. Sequential Gaussian simulation has been widely use in practice due to its simplicity and straightforwardness in a variety of areas (Alabert and Massonnat, 1990; Ravenscroft, 1994), but the accuracy of this method is not always ensured (Emery, 2004; Emery and Peláez, 2011; Gómez-Hernández and Cassiraga, 1994; Omre et al., 1993; Tran, 1994) and its applicability to multivariate cases may be challenging and require simplifications (Almeida and Journel, 1994; Gómez-Hernández and Journel, 1993). An alternative to obtain good-quality realizations is the turning bands approach proposed by Matheron (1973). In a nutshell, this method performs simulation in a multi-dimensional space through a series of one-dimensional simulations. The algorithm allows fast calculations and, in theory, yields an accurate reproduction of the spatial correlation structure (in univariate and multivariate cases), although the resulting distributions may slightly differ from the target ones due to the use of a finite number of one-dimensional simulations (stripping effect) (Emery and Lantuéjoul, 2006).

The purpose of this paper is to assess the performance and check the accuracy of sequential Gaussian and turning bands simulation, through actual and synthetic case studies.

2. Theory of joint simulation

It is often of interest to construct numerical models that reproduce the joint distribution of several coregionalized variables at unsampled locations, conditionally to the information available at sampling locations (conditional cosimulation). Because the variables are usually spatially cross-correlated, it is not sufficient to simulate each variable separately. Instead, a multivariate approach has to be used.

In the case of representing the coregionalized variables of interest by Gaussian random fields, the problem of cosimulation consists in constructing realizations of a vector Gaussian random field, say $\mathbf{Y} = \{\mathbf{Y}(\mathbf{x}): \mathbf{x} \in \mathbf{D}\}$, where $\mathbf{D}$ is the domain of interest and $\mathbf{x}$ represents a generic location in $\mathbf{D}$. For the sake of simplicity, further assume that the random field has zero mean and that its spatial correlation structure can be represented by a linear coregionalization model (Journel and Huijbregts, 1978; Wackernagel, 2003):

$$\mathbf{C}(\mathbf{h}) = \sum_{s=1}^{S} \mathbf{B}_s \, \rho_s(\mathbf{h}) \tag{1}$$

where $\{\rho_s: s = 1,\ldots, S\}$ is a set of auto-correlation functions (basic nested structures)

$\{\mathbf{B}_s: s = 1,\ldots, S\}$ is a set of real-valued, positive semi-definite matrices (coregionalization matrices)

$\mathbf{C}(\mathbf{h})$ is a matrix containing the direct (diagonal terms) and cross (off-diagonal) covariance functions of the components of $\mathbf{Y}$ for a given separation vector $\mathbf{h}$: $\mathbf{C}(\mathbf{h}) = E\{\mathbf{Y}(\mathbf{x}) \cdot \mathbf{Y}(\mathbf{x}+\mathbf{h})^{\mathrm{T}}\}$.

2.1. Sequential Gaussian cosimulation

Consider that $\mathbf{D}$ is composed of n locations: $\mathbf{D} = \{\mathbf{x}_1,\ldots, \mathbf{x}_n\}$. The sequential algorithm aims at simulating the vector random field $\mathbf{Y}$ at each location successively. Specifically, at location $\mathbf{x}_i$ (with $i = 1,\ldots, n$), the simulated vector is obtained as follows:

$$\mathbf{Y}(\mathbf{x}_i) = \mathbf{Y}^{SCK}(\mathbf{x}_i) + \sqrt{\Sigma^{SCK}(\mathbf{x}_i)}\ \mathbf{U}_i, \tag{2}$$

where

- $\mathbf{Y}^{\mathrm{SCK}}(\mathbf{x}_i)$ is the simple cokriging prediction of $\mathbf{Y}(\mathbf{x}_i)$, obtained by using the pre-existing data as well as $\mathbf{Y}(\mathbf{x}_1),\ldots, \mathbf{Y}(\mathbf{x}_{i-1})$ as conditioning data
- $\boldsymbol{\Sigma}^{\mathrm{SCK}}(\mathbf{x}_i)$ is the variance-covariance matrix of the associated cokriging errors
- $\sqrt{\Sigma^{SCK}(\mathbf{x}_i)}$ is the principal square root of $\boldsymbol{\Sigma}^{\mathrm{SCK}}(\mathbf{x}_i)$ (alternatively, the Cholesky factor of $\boldsymbol{\Sigma}^{\mathrm{SCK}}(\mathbf{x}_i)$ could be used instead of the principal square root)
- $\mathbf{U}_i$ is a standard Gaussian vector with independent components, independent of $\mathbf{U}_1,\ldots, \mathbf{U}_{i-1}$.

The sequential approach is applicable to simulate any vector Gaussian random field, even when its correlation structure is not a linear coregionalization model Eq. (1) (Marcotte, 2012), and, at least in theory, is perfectly accurate. However, in practice, some simplifications are required because the cokriging is computationally prohibitive when the number of data is too large. This happens when either the number of pre-existing data or the number of locations targeted for simulation (n) is large. In this context, the following approximations are often used.

2.1.1. Full cokriging in a moving neighborhood

Instead of cokriging with all the previously simulated vectors $\mathbf{Y}(\mathbf{x}_1),\ldots, \mathbf{Y}(\mathbf{x}_{i-1})$ and all the pre-existing conditioning data, one can restrict to the vectors and data that are located in a neighborhood of the target point $\mathbf{x}_i$. The design of such a neighborhood often considers a maximal search radius around the target point, as well as the definition of a maximum number of data and previously simulated vectors to search for (Deutsch and Journel, 1998; Goovaerts, 1997; Pebesma, 2004). The use of a local neighborhood is often combined with a multiple-grid strategy, which consists in visiting the target grid nodes according to a set of nested grids (starting from a coarse grid and following with finer ones), in order to better reproduce the spatial correlation at different scales (Tran, 1994).

2.1.2. Collocated cokriging in a moving neighborhood

Here, simulation is performed in a hierarchical manner: the first component of $\mathbf{Y}$ is simulated first, using univariate kriging in a moving neighborhood to determine the successive simulated values. The second component of $\mathbf{Y}$ is then simulated using cokriging, conditionally to the