Statistical tests for validating geostatistical simulation algorithms ☆

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A B S T R A C T

Geostatistical simulation relies on the definition of a stochastic model (e.g. a random field characterized by the set of its finite-dimensional distributions), a spatial domain and an algorithm used to construct realizations of the model over the domain. In practice, most algorithms are approximate, because their implementation requires simplifications or because the convergence to the model is only asymptotic. This work addresses the problem of evaluating the ability of a given algorithm to reproduce the underlying model. Several statistical tests are proposed in order to detect whether the fluctuations observed between the sample statistics (in particular, the spatial average, variance and regional semi-variogram) and the associated theoretical statistics (mean value, dispersion variance and semi-variogram) are inconsistent with the random field model and domain size. The tests are illustrated on a few examples and a set of computer programs is provided.

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Random field
Ergodic fluctuation
Student's test
Hotelling's test
Chi-squared test
Regional semi-variogram

1. Introduction

Geostatistical simulation is used to predict complex transfer functions and to quantify uncertainty in a spatial context, and has found acceptance in mineral resources evaluation, reservoir characterization, hydrology, soil and environmental sciences, to cite a few application domains. Its implementation relies on three components:

(1) A stochastic *model*, which is characterized by a probability space (Ω,A,P), where Ω is the set of possible realizations, A is a σ-algebra on Ω (set of events) and P is a probability on A. Models differ by their type (random field, random set, population of objects, point process,…), parameters, and also by the possible presence of conditioning data. For random fields (which is the case of interest in this work), the model contains information on its finite-dimensional distributions and reflects the spatial dependence structure.

(2) A *domain* corresponding to the portion of space (set of locations) where the model has to be simulated.

(3) An *algorithm*, which is the particular mechanism used to construct realizations of the model over the domain of interest. For example, to simulate Gaussian random fields, i.e. random fields with multivariate normal distributions, one can resort to the matrix decomposition (Davis, 1987), circulant-embedding (Dietrich and Newsam, 1993), sequential Gaussian (Ripley, 1987) or turning bands (Matheron, 1973) algorithms, to cite a few options. Although the first two algorithms yield exact simulations of the target random field, they are restricted on the number or on the spatial configuration of the locations where simulation is performed. As for the other algorithms, their practical implementation requires approximations, such as moving neighborhood restrictions (sequential Gaussian) or the use of a finite number of lines (turning bands). Accordingly, it is essential to assess the impact of such approximations on the quality of the algorithm.

This work is not concerned with testing the consistency between a set of experimental data and an assumed stochastic model. Instead, it addresses the problem of

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assessing the correctness of an algorithm for simulating a given random field model in a given domain. The objective is to propose some statistical tests and computer programs for validating the algorithm and to illustrate them on a few examples.

2. How to validate a simulation algorithm?

One approach to validating geostatistical simulation is to perform cross-validation or jackknife against a set of data (or, in some cases, against exhaustive datasets) and to check the accuracy of transfer function predictions and of the uncertainty models (Gotway and Rutherford, 1994; Deutsch, 1997). For instance, in mining applications, one can think of using exploration data to predict production data. This approach does not test for the sole simulation algorithm, but also for the suitability of the underlying stochastic model to the data. In particular, a failure of the validation does not necessarily mean that the algorithm is deficient, as it may indicate that the model has to be revised.

A second approach consists in comparing the multivariate distributions (or, at least, some of its moments) of the simulated random field with those of the model. However, in general, the calculations of multivariate distributions are intractable analytically, so that theoretical results are available for a few specific cases only. In this respect, studies on the turning bands algorithm have been presented by Mantoglou and Wilson (1982), Tompson et al. (1989), Freulon and de Fouquet (1991), Lantuéjoul (1994) and Gneiting (1999). However, the recommendations given by these authors for the practical implementation of the algorithm (choice of the number of lines) are quite different, so that the validation still remains subjective.

An alternative approach to validate the quality of a simulation algorithm is to check the agreement between the experimental statistics of the simulated random field (e.g. the mean, semi-variogram and indicator semi-variograms calculated over several realizations) and the corresponding model statistics. As an example, applications of this procedure to the sequential Gaussian algorithm have been presented by Omre et al. (1993), Gómez-Hernández and Cassiraga (1994), Tran (1994), Leuangthong et al. (2004) and Emery (2004).

The comparison of experimental and model statistics may, however, be misleading. Indeed, given that the domain in which the random field is simulated is not infinite, one always observes a departure or "fluctuation" between both types of statistics (Matheron, 1965). Based on this notion, the idea developed in this article is to validate a simulation algorithm by checking that the observed fluctuations are consistent with the random field model and with the size of the domain where simulation is performed. So far, the inspection of such fluctuations is not systematic in geostatistical simulation studies, although it has been advocated by Lantuéjoul (1994), Chilès and Delfiner (1999), Emery (2004) and Emery and Lantuéjoul (2006).

3. Definition of statistical tests

Let Y be a random field in R^d satisfying the following properties:

(1) stationarity: the finite-dimensional distributions are invariant under spatial translation;
(2) finiteness of its moments, at least up to the fourth order;
(3) strong mixing: for any domains D and D' in R^d, one has (Rosenblatt, 1985)

$$\sup_{A\in A_1,\ A'\in A_2} |P(A\cap A') - P(A)P(A')| \leqslant \phi(d(D,D')), \qquad (1)$$

where A_1 and A_2 are the σ-algebras generated by the sets of random variables $\{Y(\mathbf{x}), \mathbf{x}\in D\}$ and $\{Y(\mathbf{x}'), \mathbf{x}'\in D'\}$, respectively, $d(D,D') = \inf_{\mathbf{x}\in D\ \mathbf{x}'\in D'} |\mathbf{x}-\mathbf{x}'|$ is the Euclidian distance between D and D', and ϕ is a function such that $\phi(d)\to 0$ as $d\to\infty$.

The strong mixing property will be useful to assume that spatial averages calculated over large domains have approximately normal distributions, by virtue of a generalization of the central limit theorem (Bolthausen, 1982). For a stationary Gaussian random field, a sufficient condition for this property to hold is that the covariance function has a positive continuous spectral density (Rosenblatt, 1985). This excludes covariance functions that do not tend to zero at infinity or that have a sinusoidal component (in both cases, the spectral measure has an atom and the spectral density is undefined), as well as covariance functions that decay slowly at large lags and have infinite *integral ranges* (in such cases, the spectral density is singular in the neighborhood of zero). For most geostatistical applications, strong mixing can be assumed when the covariance function of Y is absolutely integrable in R^d, i.e. when the integral range exists and is finite (Lantuéjoul, 1991). This is the case when the covariance function has a finite range (e.g. a spherical model) or when it vanishes rapidly as the norm of the lag vector tends to infinity (e.g. an exponential or a Gaussian model).

Let m denote the mean value (expectation) of Y, C its covariance function, γ its semi-variogram and D a finite domain of R^d in which Y has to be simulated. In the following, we will examine the fluctuations in the experimental first- and second-order moments of Y around the corresponding theoretical parameters. For the sake of simplicity, the tests are performed on non-conditional realizations, since the distributions of a random field conditioned to data differ from its prior distributions and are generally hard to determine analytically (Appendix A).

3.1. Testing the reproduction of the mean value and dispersion variance

The average of the random field Y over domain D, denoted by $Y(D)$ hereunder, is a random variable with the same expectation (m) as Y. Because of the mixing property, and provided that D is large with respect to

the integral range, one can assume that $Y(D)$ has a normal distribution (Bolthausen, 1982; Rosenblatt, 1985).

Let $\bar{Y}(D)$ and $S^2_{Y(D)}$ be the sample mean and sample variance of N realizations of $Y(D)$ drawn independently. Then

$$\frac{\overline{Y}(D)-m}{S_{Y(D)}}\sqrt{N-1}\sim T_{N-1}, \tag{2}$$

where T_{N-1} is a Student random variable with $N-1$ degrees of freedom and $\sim$ indicates an equality of the distributions. Formula (2) allows deriving an interval with a pre-specified probability (say, $1-\alpha=0.95$) of finding $\overline{Y}(D)$. If the actual value of $\overline{Y}(D)$ does not belong to this interval, the simulation algorithm should be questioned.

A Student test can also be designed for the dispersion of the simulated values within domain D. Specifically, let $s^2(\circ|D)$ denote the sample variance of the random field Y over D; this is a random variable whose expectation is the dispersion variance in D

$$\sigma^2(\circ|D)=\frac{1}{|D|^2}\int_D\int_D \gamma(\mathbf{x}'-\mathbf{x})\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}', \tag{3}$$

where $|D|$ stands for the measure of D.

Let $\overline{s^2}(\circ|D)$ and $S^2_{s^2(\circ|D)}$ be the mean and variance of N realizations of $s^2(\circ|D)$. Then

$$\frac{\overline{s^2}(\circ|D)-\sigma^2(\circ|D)}{S_{s^2(\circ|D)}}\sqrt{N-1}\sim T_{N-1}. \tag{4}$$

3.2. Testing the reproduction of the semi-variogram at a given lag

The regional semi-variogram over D for a given lag vector $\mathbf{h}\in R^d$ is defined as

$$\Gamma_D(\mathbf{h})=\frac{1}{2K_{\mathbf{h}}(\mathbf{0})}\int_{D\cap D_{-\mathbf{h}}}[Y(\mathbf{x}+\mathbf{h})-Y(\mathbf{x})]^2\,\mathrm{d}\mathbf{x}, \tag{5}$$

where $D_{-\mathbf{h}}$ represents domain D shifted by vector $-\mathbf{h}$ and $K_{\mathbf{h}}$ is the geometric covariogram of $D\cap D_{-\mathbf{h}}$; in particular, $K_{\mathbf{h}}(\mathbf{0})$ is the measure of $D\cap D_{-\mathbf{h}}$. The expected value of $\Gamma_D(\mathbf{h})$ is the semi-variogram model at lag $\mathbf{h}$, i.e. $\gamma(\mathbf{h})$, and (provided that $D\cap D_{-\mathbf{h}}$ is large with respect to the integral range) its distribution is close to normal, according to the central limit theorem for mixing random fields (Davis and Borgman, 1982).

Let $\overline{\Gamma}_D(\mathbf{h})$ and $S^2_{\Gamma_D(\mathbf{h})}$ be the sample mean and sample variance of the regional semi-variograms calculated over N realizations of Y. It comes

$$\frac{\overline{\Gamma}_D(\mathbf{h})-\gamma(\mathbf{h})}{S_{\Gamma_D(\mathbf{h})}}\sqrt{N-1}\sim T_{N-1}, \tag{6}$$

which allows constructing an interval for $\overline{\Gamma}_D(\mathbf{h})$ with a pre-specified probability $1-\alpha$.

3.3. Testing the reproduction of the semi-variogram at multiple lags

A question that naturally arises is the determination of a region with probability $1-\alpha$ for the average regional semi-variogram calculated at several lags $\mathbf{h}_1,\ldots,\mathbf{h}_K$. One possibility is to consider an interval with probability $1-\alpha/K$ for each lag, according to Bonferroni's inequality. However, this approach does not take into account the stochastic dependence between the regional semi-variograms at lags $\mathbf{h}_1,\ldots,\mathbf{h}_K$ and may therefore fail to detect significant results.

To get out of this problem, assume that $\mathbf{\Gamma}_D=(\Gamma_D(\mathbf{h}_1),\ldots,\Gamma_D(\mathbf{h}_K))^{\mathrm{T}}$ has a multivariate normal distribution, with mean vector $\boldsymbol{\gamma}=(\gamma(\mathbf{h}_1),\ldots,\gamma(\mathbf{h}_K))^{\mathrm{T}}$ (Pardo-Igúzquiza and Dowd, 2001). Let $\overline{\mathbf{\Gamma}}_D$ and $\mathbf{S}^2_{\mathbf{\Gamma}_D}$ denote the sample mean vector and sample variance–covariance matrix of $\mathbf{\Gamma}_D$, calculated over N realizations of Y. Then one has

$$(N-1)(\overline{\mathbf{\Gamma}}_D-\boldsymbol{\Upsilon})^{\mathrm{T}}(\mathbf{S}^2_{\overline{\mathbf{\Gamma}}_D})^{-1}(\overline{\mathbf{\Gamma}}_D-\boldsymbol{\Upsilon})\sim T^2_{N,K}, \tag{7}$$

where $T^2_{N,K}$ is a Hotelling random variable, proportional to a Fisher random variable $F_{K,N-K}$ with K and N–K degrees of freedom:

$$T^2_{N,K}=\frac{K(N-1)}{N-K}F_{K,N-K}. \tag{8}$$

Eq. (7) can be seen as a multivariate generalization of Eq. (6), as the square of a Student random variable with $N-1$ degrees of freedom is a Fisher random variable with 1 and $N-1$ degrees of freedom.

3.4. Testing the dispersion of the regional semi-variogram

The above Student and Hotelling's tests allow checking whether there exists a bias in the reproduction of the semi-variogram model, either at a single lag or at multiple lags simultaneously. In this subsection, we will examine the dispersion of the regional semi-variogram around the prior model. Again, assuming that the regional semi-variogram at lag $\mathbf{h}$ is normally distributed, it comes

$$\frac{NS^2_{\Gamma_D(\mathbf{h})}}{\mathrm{var}[\Gamma_D(\mathbf{h})]}\sim\chi^2_{N-1}, \tag{9}$$

where χ^2_{N-1} is a chi-squared random variable with $N-1$ degrees of freedom. From this, one can define a two-sided test to detect whether the actual variance of the regional semi-variogram is significantly smaller or greater than that of the model.

This test can also be extended to validating the joint dispersion of the regional semi-variogram at several lags $\mathbf{h}_1,\ldots,\mathbf{h}_K$. Let us use the same notations as in Section 3.3 and introduce the theoretical variance–covariance matrix $\mathbf{\Sigma}^2_D$ of vector $\mathbf{\Gamma}_D$. Then

$$\sum_{n=1}^{N}\{(\mathbf{\Gamma}_D^{(n)}-\overline{\mathbf{\Gamma}}_D)^{\mathrm{T}}(\mathbf{\Sigma}^2_D)^{-1}(\mathbf{\Gamma}_D^{(n)}-\overline{\mathbf{\Gamma}}_D)\}\sim\chi^2_{K(N-1)} \tag{10}$$

in which $\mathbf{\Gamma}_D^{(n)}$ is the regional semi-variogram vector calculated over the nth realization of Y.

The expression of the covariance of $\mathbf{\Gamma}_D$ depends on the quadrivariate distributions of the simulated random field Y. A simple example is that of a stationary Gaussian random field, for which one has (Matheron, 1989)

$$\begin{aligned}&\mathrm{cov}\{[Y(\mathbf{x}+\mathbf{h})-Y(\mathbf{x})]^2,[Y(\mathbf{x}'+\mathbf{h}')-Y(\mathbf{x}')]^2\}\\&\quad=2[\gamma(\mathbf{x}-\mathbf{x}'+\mathbf{h})+\gamma(\mathbf{x}-\mathbf{x}'-\mathbf{h}')-\gamma(\mathbf{x}-\mathbf{x}')\\&\qquad-\gamma(\mathbf{x}-\mathbf{x}'+\mathbf{h}-\mathbf{h}')]^2.\end{aligned} \tag{11}$$

This entails

$$\begin{aligned}\mathrm{var}[\Gamma_D(\mathbf{h})] &= \frac{1}{2K_{\mathbf{h}}^2(\mathbf{0})}\int_{D\cap D_{-\mathbf{h}}}\int_{D\cap D_{-\mathbf{h}}}[\gamma(\mathbf{x}-\mathbf{x}'+\mathbf{h}) \\ &\quad +\gamma(\mathbf{x}-\mathbf{x}'-\mathbf{h})-2\gamma(\mathbf{x}-\mathbf{x}')]^2\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}' \\ &= \frac{1}{2K_{\mathbf{h}}^2(\mathbf{0})}\int[\gamma(\mathbf{u}+\mathbf{h})+\gamma(\mathbf{u}-\mathbf{h}) \\ &\quad -2\gamma(\mathbf{u})]^2K_{\mathbf{h}}(\mathbf{u})\mathrm{d}\mathbf{u}. \end{aligned} \tag{12}$$

The last equality has been obtained from the first one by applying Cauchy algorithm (Chilès and Delfiner, 1999). More generally, the entries of $\mathbf{\Sigma}_D^2$ are given by

$$\begin{aligned}&\mathrm{cov}[\Gamma_D(\mathbf{h}),\Gamma_D(\mathbf{h}')] \\ &= \frac{\int[\gamma(\mathbf{u}+\mathbf{h})+\gamma(\mathbf{u}-\mathbf{h}')-\gamma(\mathbf{u})-\gamma(\mathbf{u}+\mathbf{h}-\mathbf{h}')]^2K_{\mathbf{h};\mathbf{h}'}(\mathbf{u})\,\mathrm{d}\mathbf{u}}{2K_{\mathbf{h}}(\mathbf{0})K_{\mathbf{h}'}(\mathbf{0})}\end{aligned} \tag{13}$$

where $K_{\mathbf{h};\mathbf{h}'}$ is the geometric cross-covariogram between $D\cap D_{-\mathbf{h}}$ and $D\cap D_{-\mathbf{h}'}$

$$K_{\mathbf{h};\mathbf{h}'}(\mathbf{u}) = \mathit{measure}\{D\cap D_{-\mathbf{h}'}\cap D_{-\mathbf{u}}\cap D_{-\mathbf{u}-\mathbf{h}}\}. \tag{14}$$

Other examples of random field models for which the (co)variance of the regional semi-variogram can be expressed analytically are given by Alfaro (1979) and Emery (2005).

3.5. Comments

Before going through examples, several comments are worthwhile:

(1) The tests indicate whether there is a statistical evidence for rejecting the hypothesis of an accurate reproduction of the random field model. The acceptation of a test does not necessarily mean that the simulation algorithm is correct; rather it means that there is no significant proof of the contrary. In contrast, the rejection of the test is a stronger conclusion, as the probability of a false positive (type I error) is less than α (*significance level* of the test).

(2) The tests on the semi-variogram (Sections 3.2–3.4) actually require an assumption of intrinsic stationarity for Y, i.e. that the distributions of its increments (rather than of the random field itself) are invariant under spatial translation and have finite moments.

(3) Concerning these tests, the choice of the lag vectors is free and can be made according to the application under consideration. For instance, small vectors would be adequate if one wants to regularize the realizations and to determine block support distributions (e.g. in mining engineering, to calculate the recoverable resources at a selective mining unit support). In contrast, if one is concerned with the response to a transfer function that involves the whole field (e.g. in petroleum reservoir modeling, a flow simulation so as to assess the uncertainty in production variables), it is also advisable to test the semi-variogram reproduction at large lags.

(4) *Multiple testing problem*. To assess a simulation algorithm, one may be interested in testing several realization statistics (mean, variance, semi-variogram, etc.). In such a case, to obtain an overall significance level equal to α' (probability of type I error), the level α for each test must be chosen smaller. In particular, if K tests are performed over independent statistics, then the overall significance level is given by

$$\alpha' = 1-(1-\alpha)^K. \tag{15}$$

For instance, this is the case if one considers a test on the mean and a test on the semi-variogram, since the latter only depends on the increments of the random field and is therefore not affected by the mean. In the general case where the tests statistics are not independent, one has (Bonferroni's inequality)

$$\alpha' \leqslant K\alpha. \tag{16}$$

However, this inequality is conservative and results in an overstatement of the true significance level when the test statistics are strongly dependent. This situation has been discussed when testing the reproduction of the semi-variogram at several lags, for which a Hotelling test should be considered instead of several Student tests performed separately (Eqs. (6) and (7)). A simple way to get out of the multiple testing problem is to carry out each test on a different set of realizations of the random field: the test statistics are therefore independent and one can resort to Eq. (15) to calculate the overall significance level.

(5) A given simulation algorithm may successfully pass some tests and fail at other tests. For instance, it can accurately reproduce the univariate distribution of the random field (hence, the mean value), but not the semi-variogram. In such a situation, it behooves the practitioner to decide whether the statistics that fail to be validated are essential or not to the solution of the problem at hand.

(6) The size of the simulation domain has an impact on the magnitude of the fluctuations between experimental and model statistics (Matheron, 1965): the larger the domain, the smaller the fluctuations, so that inaccurate simulation algorithms are more likely to be detected (it is easier to identify a bias when fluctuations are negligible). Conversely, when the simulation is performed on a small domain, the algorithms are more likely to pass the tests because fluctuations may hide possible biases.

(7) The tests assume that the simulation domain D is much larger than the integral range, so that the experimental statistics calculated over a realization (sample mean, sample variance, regional semi-variogram at a given lag) are almost normally distributed. This assumption can be checked by plotting the quantiles of the statistics obtained over a set of realizations against the normal quantiles. As a rule of thumb, Tompson et al. (1989) suggest that

the size of the simulation domain in any direction should be larger than 10 times the correlation range in the same direction.

(8) Student and Hotelling's tests are robust against departures from normality and can be used even if domain D is not large with respect to the integral range. Also, they can be generalized to detect biases in the reproduction of other statistics, such as the indicator semi-variograms associated with given thresholds or the semi-variograms of order less than 2 (semi-madogram, semi-rodogram, etc.).

(9) The chi-squared test on the regional semi-variogram (Eq. 9) is more demanding, as its validity is ensured only if the regional semi-variogram has a normal distribution (see comment no. 6). The application of this test should therefore be restricted to small lags and large simulation domains (Davis and Borgman, 1982). Otherwise one can perform the test on the average semi-variogram of a group of M realizations, instead of the semi-variogram of a single realization

$$\frac{NS^2_{\overline{\Gamma}_D(\mathbf{h})}}{\mathrm{var}[\overline{\Gamma}_D(\mathbf{h})]} \sim \chi^2_{N-1}, \tag{17}$$

where $\overline{\Gamma}_D$ is the average regional semi-variogram of a group of M realizations and N is the number of such groups (i.e. $N \times M$ realizations are drawn in total). If M is large, the distribution of $\overline{\Gamma}_D(\mathbf{h})$ is normal (central limit theorem).

(10) The chi-squared test proposed in Eq. (10) relies on an even stronger assumption of multivariate normality for the regional semi-variogram at multiple lags, which can be unwarranted in practice. Indeed, a weighted average of the components of $\mathbf{\Gamma}_D$ is a sum of non-identically distributed and correlated random variables and may therefore not have a Gaussian distribution (the central limit theorem may not apply). Again, to avoid this inconvenient, the test can be done on the average regional semi-variogram of a group of M realizations.

(11) The aforementioned tests are implemented in a set of Matlab programs (version 5.0 or later) provided together with this article. The reader is referred to the headers of the program files for a description of the input and output parameters:

- **STUDENT_MEAN.M**: Student's test on the mean (Eq. (2)).
- **STUDENT_VAR.M**: Student's test on the variance (Eq. (4)).
- **STUDENT_VARIOG.M**: Student's test on the semi-variogram at a single lag (gridded realizations) (Eq. (6))
- **HOTELLING_VARIOG.M**: Hotelling's test on the semi-variogram at multiple lags (gridded realizations) (Eq. (7))
- **CHI2_VARIOG.M**: chi-squared test on the dispersion of regional semi-variogram at a single lag (gridded realizations; multivariate normal model) (Eqs. (9)–(12)).

4. Applications

4.1. Simulating a Gaussian random field with the sequential algorithm

Let us consider the sequential algorithm (Ripley, 1987) for constructing realizations of a stationary Gaussian random field with an isotropic semi-variogram with sill 1 and range 40 over a $400 \times 400 \times 1$ regular grid in R^3. A key aspect in the implementation of the algorithm is the number of neighboring data used for conditioning kriging, as a unique neighborhood implementation is impractical. In the following, four moving neighborhoods are considered, containing up to 10, 20, 50 and 100 conditioning data, respectively, and three isotropic semi-variogram models (spherical, exponential and Gaussian, the latter with a 0.5% of relative nugget effect) are put to the tests. In each case, a random path is used to visit the nodes of the simulation grid and a spiral search is performed to select the data closest to the node under consideration (Gómez-Hernández and Cassiraga, 1994).

The test on the spatial averages of 100 realizations does not allow rejecting any of the implementations, as the absolute values of the Student statistics are always below the critical values (1.984) for a 95% probability (Table 1). This is explained because the sequential algorithm reproduces the univariate distribution of the Gaussian random field, irrespective of the number of conditioning data considered in the moving neighborhood (Emery, 2004). However, with the first implementation (10 conditioning data), the sample variance does not match the theoretical dispersion variance in the cases of the exponential and Gaussian semi-variogram models, which suggests that the spatial correlation of the random field is not accurately reproduced.

Furthermore, Student's and Hotelling's tests on the regional semi-variograms indicate a bias in the reproduction of the semi-variogram model, unless the latter is an exponential model and the neighborhood contains at least 50 conditioning data (Table 1 and Fig. 1). Concerning the dispersion of the regional semi-variograms, the chi-squared test also casts doubt on the validity of the first two implementations (with 10 and 20 conditioning data) in the cases of the spherical and exponential semi-variogram models.

4.2. Simulating a Gaussian random field with a continuous spectral algorithm

An alternative to the sequential algorithm is to simulate a Gaussian field by adding independent random fields $\{Y_j,\ j = 1, \ldots, J\}$ with the same finite-dimensional distributions (Lantuéjoul, 1994)

$$\forall \mathbf{x} \in R^d,\ Y^{(J)}(\mathbf{x}) = \frac{1}{\sqrt{J}} \sum_{j=1}^{J} Y_j(\mathbf{x}). \tag{18}$$

According to the central limit theorem, the finite-dimensional distributions of $Y^{(J)}$ tend to that of a Gaussian random field as J tends to infinity. Let $\Gamma_{D,J}$ be the regional semi-variogram of $Y^{(J)}$, $\Gamma_{D,1}$ the regional semi-variogram of

Table 1
Statistical tests on 100 sequential Gaussian realizations over a $400 \times 400 \times 1$ grid

Number of conditioning data	Absolute value of statistics			95% probability interval	
	Spherical semi-variogram	Exponential semi-variogram	Gaussian semi-variogram	Lower bound	Upper bound
Student's test on mean value					
10	0.868	0.996	0.784	0	1.984
20	0.870	0.978	0.909	0	1.984
50	0.880	0.985	0.955	0	1.984
100	0.893	0.985	0.975	0	1.984
Student's test on variance					
10	1.751	**2.991**	**2.393**	0	1.984
20	0.491	0.128	0.215	0	1.984
50	1.066	0.636	1.163	0	1.984
100	1.166	0.663	1.289	0	1.984
Student's test on semi-variogram (lag distance = 10)					
10	**26.99**	**30.30**	**17.75**	0	1.984
20	**9.58**	**11.97**	**8.649**	0	1.984
50	0.008	0.136	**2.356**	0	1.984
100	0.746	0.626	0.306	0	1.984
Hotelling's test on semi-variogram (lag distances = 10, 20, 30, 40, 50)					
10	**2104**	**1565**	**7982**	0	12.04
20	**536.8**	**243.2**	**2505**	0	12.04
50	**107.7**	3.34	**556.1**	0	12.04
100	**32.41**	2.67	**157.3**	0	12.04
Chi-squared test on semi-variogram (lag distance = 10)					
10	**61.03**	**69.61**	81.39	73.36	128.42
20	**70.65**	**72.39**	104.13	73.36	128.42
50	78.78	76.88	103.61	73.36	128.42
100	79.54	77.32	105.35	73.36	128.42

Simulated random field has an isotropic semi-variogram with sill 1 and practical range 40 units. Semi-variograms are calculated along abscissa axis. Bold numbers correspond to situations for which there is evidence that simulation algorithm fails.

the basic random field Y_1, and $\Gamma_{D,\infty}$ the regional semi-variogram of the asymptotical Gaussian random field. Then, it can be shown (Appendix B) that the fluctuation variance of $\Gamma_{D,J}$ is

$$\mathrm{var}[\Gamma_{D,J}(\mathbf{h})] = \left(1 - \frac{1}{J}\right)\mathrm{var}[\Gamma_{D,\infty}(\mathbf{h})] + \frac{1}{J}\mathrm{var}[\Gamma_{D,1}(\mathbf{h})]. \quad (19)$$

This formula indicates that the fluctuation variance of the regional semi-variogram of $Y^{(J)}$ is not the same as that of a Gaussian random field, but the bias gets smaller as J increases. In practice, J is on the order of several hundreds or several thousands, so that the variance of $\Gamma_{D,J}(\mathbf{h})$ should be close to that of $\Gamma_{D,\infty}(\mathbf{h})$, unless the latter is much smaller that the variance of $\Gamma_{D,1}(\mathbf{h})$. This circumstance may happen when the norm of $\mathbf{h}$ is close to zero (Alfaro, 1979; Matheron, 1989), as it will be seen hereunder.

As an application of formula (19), let us consider the simulation of a random field with covariance function C by means of a continuous spectral method (Shinozuka, 1971; Lantuéjoul, 1994). This method consists in putting

$$\forall \mathbf{x} \in R^d,\ \forall j \in \{1, \ldots, J\},\ Y_j(\mathbf{x}) = \sqrt{2}\cos(\langle \boldsymbol{\Omega}_j, \mathbf{x}\rangle + \Phi_j), \quad (20)$$

where $\langle , \rangle$ is the standard inner product in R^d, $\boldsymbol{\Omega}_j$ is a random vector whose distribution is the spectral measure of C, and Φ_j is an independent uniform random variable in $[0,2\pi)$. After some calculations, one finds the following expression for the fluctuation variance of the regional semi-variogram of Y_1 at lag $\mathbf{h}$:

$$\mathrm{var}\{\Gamma_{D,1}(\mathbf{h})\} = \frac{1}{2K_{\mathbf{h}}^2(\mathbf{0})} E\left\{\sin^4\left(\frac{\langle \boldsymbol{\Omega}_1, \mathbf{h}\rangle}{2}\right) \times \int [2\cos^2(\langle \boldsymbol{\Omega}_1, \mathbf{u}\rangle) + 1] K_{\mathbf{h}}(\mathbf{u})\, d\mathbf{u}\right\} - \gamma^2(\mathbf{h}). \quad (21)$$

The expected value in this expression can be calculated by Monte Carlo integration.

Table 2 gives the ratio between the variance of $\Gamma_{D,J}(\mathbf{h})$ and that of $\Gamma_{D,\infty}(\mathbf{h})$ for several lag vectors and for several values of J, when simulating a random field with an isotropic exponential or Gaussian semi-variogram over a $400 \times 400 \times 1$ domain in R^3. The results suggest that the convergence of $Y^{(J)}$ to a Gaussian random field is faster when the semi-variogram is smooth at the origin (Gaussian semi-variogram), which has already be pointed out by Lantuéjoul (2002, p. 192).

A numerical exercise made on 100 realizations confirms that the fluctuation variance is well reproduced when J is set to 10,000 (Table 3). Besides, Hotelling's test for the same lag vectors gives a $T^2_{99,5}$ statistics of 4.25 and 3.43 for the exponential and Gaussian semi-variograms,

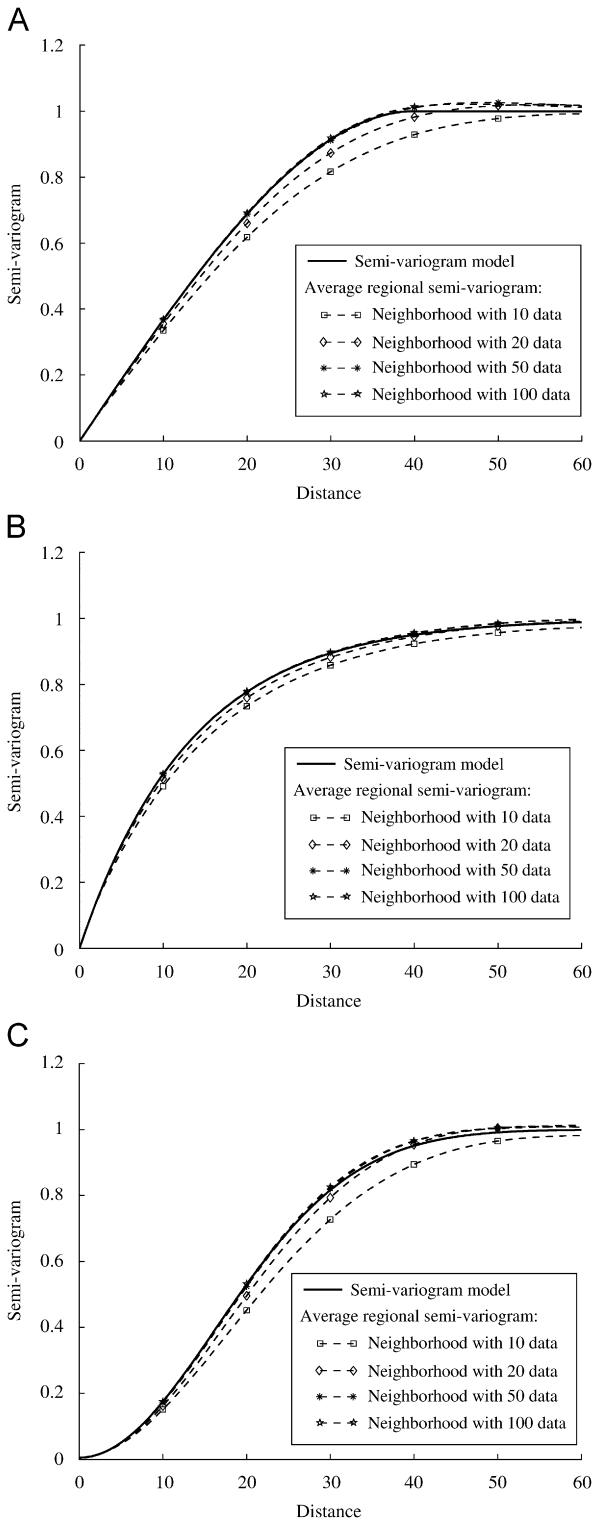

Fig. 1. Semi-variogram model (solid line) and average regional semi-variograms (dashed lines) of 100 sequential Gaussian realizations over a $400 \times 400 \times 1$ grid. Simulated random field has an isotropic spherical (A), exponential (B) and Gaussian (C) semi-variogram with sill 1 and range 40 units. Semi-variograms are calculated along abscissa axis.

Table 2
Ratio of fluctuation variance of regional semi-variogram obtained with continuous spectral algorithm and fluctuation variance of a Gaussian random field over a $400 \times 400 \times 1$ grid

	Norm of lag vector				
	10	20	30	40	50
Exponential semi-variogram					
$J = 1$	1819	425	207	143	115
$J = 10$	183	43.4	21.6	15.2	12.4
$J = 100$	19.2	5.24	3.06	2.42	2.14
$J = 1000$	2.82	1.42	1.21	1.14	1.11
$J = 10{,}000$	1.18	1.04	1.02	1.01	1.01
Gaussian semi-variogram					
$J = 1$	213	121	67.8	44.5	34.8
$J = 10$	22.2	13.0	7.68	5.35	4.38
$J = 100$	3.12	2.20	1.67	1.44	1.34
$J = 1000$	1.21	1.12	1.07	1.04	1.03
$J = 10{,}000$	1.02	1.01	1.01	1.00	1.00

Simulated random field has an isotropic semi-variogram with practical range 40 units. Lag vector is oriented along abscissa axis.

respectively, therefore no bias is detected in the reproduction of the prior model (the critical $T^2_{99,5}$ value is 12.04).

4.3. Simulating a dead leaves random field

We now consider the simulation of a dead leaves model over a $400 \times 400 \times 1$ grid in R^3. This model relies on a homogeneous Poisson point process in $R^3 \times R_+$ (space-time), at each point of which a random set called *primary grain* is seeded. In the present case, the primary grain is chosen as a ball whose diameter is uniformly distributed in (0,120). Each grain has a constant valuation (a standard normal random variable) that is independent of the valuations of the other grains. At any location in R^3, the value of the random field can be defined in two equivalent fashions (Matheron, 1968; Jeulin, 1997):

(i) consider the value of the first primary grain that covers this location and
(ii) consider the value of the last primary grain that covers this location.

It can be shown that the dead leaves random field has the following semi-variogram:

$$\forall \mathbf{h} \in R^3, \gamma(\mathbf{h}) = \frac{2K(\mathbf{0}) - 2K(\mathbf{h})}{2K(\mathbf{0}) - K(\mathbf{h})}, \tag{22}$$

where K is the geometric covariogram of the primary grains (uniform mixture of spherical covariograms)

$$\forall \mathbf{h} \in R^3, K(\mathbf{h}) = \int_{|\mathbf{h}|}^{120} \frac{\pi a^3}{6} \left(1 - \frac{3}{2}\frac{|\mathbf{h}|}{a} + \frac{1}{2}\frac{|\mathbf{h}|^3}{a^3}\right) \mathrm{d}a. \tag{23}$$

In this exercise, we will stop the simulation once the $400 \times 400 \times 1$ grid is completely covered by primary grains. This construction is exact when retaining at each location the first grain, as the newer grains do not alter the simulated field any more. However, it is approximate

Table 3
Chi-squared test on dispersion of regional semi-variograms of 100 realizations obtained with continuous spectral algorithm ($J = 10{,}000$) over a $400 \times 400 \times 1$ grid

Norm of lag vector	χ^2_{99} statistics		Lower χ^2_{99} bound (2.5% probability)	Upper χ^2_{99} bound (97.5% probability)
	Exponential semi-variogram	Gaussian semi-variogram		
10	88.56	99.54	73.36	128.42
20	92.10	95.95	73.36	128.42
30	95.22	91.63	73.36	128.42
40	93.19	90.36	73.36	128.42
50	89.53	92.90	73.36	128.42

Simulated random field has an isotropic semi-variogram with practical range 40. Fluctuation variances are calculated for a lag vector oriented along abscissa axis.

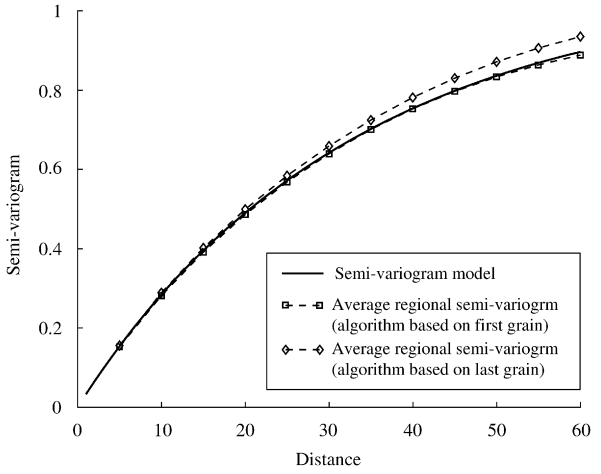

Fig. 2. Semi-variogram model (solid line) and average regional semi-variograms (dashed lines) of 100 dead leaves realizations over a $400 \times 400 \times 1$ regular grid. Primary grains are balls with uniform diameers between 0 and 120. Semi-variograms are calculated along abscissa axis.

Table 4
Hotelling's test on average regional semi-variogram of 100 dead leaves realizations over a $400 \times 400 \times 1$ grid

Convention for overlapping grains	$T^2_{99,5}$ statistics	Critical $T^2_{99,5}$ value (95% probability)
First grain	8.27	12.04
Last grain	**23.64**	12.04

Primary grains are balls with uniform diameters between 0 and 120. Semi-variograms are calculated for lag vectors oriented along abscissa axis with norms of 10, 20, 30, 40 and 50 units. Bold number corresponds to situation for which there is evidence that simulation algorithm fails.

when retaining the last grain since, in theory, the stopping time should be infinite. In particular, as pointed by Lantuéjoul (2002, p. 178), the last grain that covers the grid is likely to be bigger than the average. This approximation causes a bias in the reproduction of the semi-variogram (Fig. 2), which is detected by Hotelling's test (Table 4). In contrast, the first model successfully passes the test.

4.4. Simulating a truncated Gaussian vector with the Gibbs sampler

A question that has not been tackled so far is that of validating algorithms specific to conditional simulations, in particular iterative algorithms that are used for conditioning a large variety of random field models (e.g. Freulon, 1994; Hegstad et al., 1994; Omre and Tjelmeland, 1997; Lantuéjoul, 1997, 2002; Emery, 2007). The definition of statistical tests to validate such algorithms is arduous, as the finite-dimensional conditional distributions are often intractable from an analytical point of view. Also, the theoretical results on the rate of convergence of iterative algorithms are often scarce or impractical.

As an example, let us consider the simulation of an indicator obtained by truncating a stationary Gaussian random field in R^2. Assume that the latter has an isotropic exponential semi-variogram and that the truncation threshold is zero. Also suppose that it is of interest to condition the simulation to indicator data available at a regular 20×20 grid in R^2. A common procedure consists in simulating the Gaussian random field at the data locations with the *Gibbs sampler* (an iterative algorithm originally proposed by Geman and Geman (1984)), then simulating the Gaussian random field at other locations of R^2, and finally obtaining the indicator random field by truncation. Since Gaussian simulation algorithms have been tested in the previous subsections, here one is interested in validating the Gibbs sampler. The following approach is proposed:

(1) Draw a non-conditional simulation of the Gaussian random field over the 20×20 grid, by using the matrix decomposition method (Davis, 1987). This method is exact, so no approximation is made at this step.
(2) Truncate this field and obtain a set of indicator data over the 20×20 grid.
(3) Use the Gibbs sampler to construct Gaussian data over this grid conditioned to the previously defined

Table 5
Statistical tests on 100 Gaussian realizations over a 20×20 grid obtained with Gibbs sampler

Number of iterations	Absolute value of statistics	95% probability interval	
		Lower bound	Upper bound
Student's test on mean value			
1000	0.043	0	1.984
10,000	0.658	0	1.984
100,000	1.270	0	1.984
1,000,000	1.534	0	1.984
Student's test on variance			
1000	**4.750**	0	1.984
10,000	1.588	0	1.984
100,000	0.561	0	1.984
1,000,000	0.478	0	1.984
Student's test on semi-variogram (lag distance = 1)			
1000	**19.45**	0	1.984
10,000	1.054	0	1.984
100,000	0.416	0	1.984
1,000,000	1.416	0	1.984
Hotelling's test on semi-variogram (lag distances = 1, 2, 3, 4, 5)			
1000	**544.8**	0	12.04
10,000	4.659	0	12.04
100,000	2.354	0	12.04
1,000,000	5.574	0	12.04
Chi-squared test on semi-variogram (lag distance = 1)			
1000	**183.4**	73.36	128.42
10,000	82.01	73.36	128.42
100,000	92.51	73.36	128.42
1,000,000	123.60	73.36	128.42

Simulated random field has an isotropic exponential semi-variogram with sill 1 and range 5 units. Semi-variograms are calculated along abscissa axis. Bold numbers correspond to situations for which there is evidence that simulation algorithm fails.

indicator data. At each iteration, a datum is chosen (in this case, it is selected uniformly among all the data) and updated conditionally to the other Gaussian data.

(4) Go back to Step (1) until a sufficient number of conditional realizations are drawn.

Because the conditioning indicator data defined in Step 2 differ at each realization and are drawn from the non-conditional model, the Gaussian realizations obtained in Step 3 can be treated as if they were non-conditional. In particular, one can apply the statistical tests proposed in Section 3. The results (Table 5) indicate that the Gibbs sampler fails at reproducing the variance and semi-variogram when using as few as 1000 iterations, but is validated from 10,000 iterations onwards, which corresponds to an average of 25 updates for each datum.

5. Conclusions

In this paper, several statistical tests have been proposed for validating geostatistical simulation algorithms. Student and Hotelling's tests are robust and therefore quite general, while the chi-squared tests are applicable under more restrictive conditions. Of course, the presented tests are not exhaustive and many other tests could be designed. Since most simulation algorithms make simplifications or approximations whose impact is difficult to assess a priori, the recourse to statistical tests allow practitioners to decide on appropriate implementation parameters, e.g. the number of neighboring conditioning data to use when resorting to sequential simulation, the number of basic random fields to add when using the continuous spectral method, or the number of iterations needed for conditioning the realizations via an iterative algorithm.

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Appendix A. Expected regional semi-variogram of a conditioned Gaussian random field

Consider a stationary Gaussian random field Y with covariance function C and semi-variogram γ. Let $\{\mathbf{x}_\alpha,\ \alpha = 1, \ldots, n\}$ be the locations of conditioning data and $\{y_\alpha,\ \alpha = 1, \ldots, n\}$ the associated data values. The random field conditioned to these data can be expressed as follows (Chilès and Delfiner, 1999, p. 381):

$$\tilde{Y}(\mathbf{x}) = y_{SK}(\mathbf{x}) + \varepsilon(\mathbf{x}), \tag{A.1}$$

where $y_{SK}(\mathbf{x})$ is the simple kriging prediction of $Y(\mathbf{x})$ (a deterministic value) and $\varepsilon(\mathbf{x})$ is the simple kriging error at location $\mathbf{x}$ (a random variable with zero mean). Accordingly, for any lag vector $\mathbf{h}$, one has

$$E\{[\tilde{Y}(\mathbf{x}+\mathbf{h}) - \tilde{Y}(\mathbf{x})]^2\} = [y_{SK}(\mathbf{x}+\mathbf{h}) - y_{SK}(\mathbf{x})]^2 + E\{[\varepsilon(\mathbf{x}+\mathbf{h}) - \varepsilon(\mathbf{x})]^2\}. \tag{A.2}$$

This formula entails that the expected regional semi-variogram of the conditional random field $\tilde{Y}$ over a given domain D is equal to the regional semi-variogram of the kriging predictions plus the expected regional semi-variogram of the kriging errors. By using the following expression for the simple kriging covariance:

$$\mathrm{cov}[\varepsilon(\mathbf{x}+\mathbf{h}), \varepsilon(\mathbf{x})] = C(\mathbf{h}) - \sum_{\alpha=1}^{n}\sum_{\beta=1}^{n} \lambda_\alpha^{SK}(\mathbf{x}) \times \lambda_\beta^{SK}(\mathbf{x}+\mathbf{h}) C(\mathbf{x}_\alpha - \mathbf{x}_\beta), \tag{A.3}$$

where $\lambda_\alpha^{SK}(\mathbf{x})$ denotes the kriging weight assigned to y_α when predicting $Y(\mathbf{x})$, one finds

$$\begin{aligned} E\{[\varepsilon(\mathbf{x}+\mathbf{h}) - \varepsilon(\mathbf{x})]^2\} &= \mathrm{cov}[\varepsilon(\mathbf{x}+\mathbf{h}), \varepsilon(\mathbf{x}+\mathbf{h})] + \mathrm{cov}[\varepsilon(\mathbf{x}), \varepsilon(\mathbf{x})] - 2\mathrm{cov}[\varepsilon(\mathbf{x}+\mathbf{h}), \varepsilon(\mathbf{x})] \\ &= 2[C(\mathbf{0}) - C(\mathbf{h})] - \sum_{\alpha=1}^{n}\sum_{\beta=1}^{n} [\lambda_\alpha^{SK}(\mathbf{x}+\mathbf{h}) - \lambda_\alpha^{SK}(\mathbf{x})] \times [\lambda_\beta^{SK}(\mathbf{x}+\mathbf{h}) - \lambda_\beta^{SK}(\mathbf{x})] C(\mathbf{x}_\alpha - \mathbf{x}_\beta). \end{aligned} \tag{A.4}$$

Hence the expected value of the conditional regional semi-variogram of $\tilde{Y}$ at lag $\mathbf{h}$ is (Eqs. (A.2) and (A.4))

$$E[\tilde{\Gamma}_D(\mathbf{h})] = \gamma(\mathbf{h}) + \frac{1}{2K_{\mathbf{h}}(\mathbf{0})}\int_{D\cap D_{-\mathbf{h}}}[y_{SK}(\mathbf{x}+\mathbf{h}) - y_{SK}(\mathbf{x})]^2\,\mathrm{d}\mathbf{x} - \frac{1}{2K_{\mathbf{h}}(\mathbf{0})}\int_{D\cap D_{-\mathbf{h}}}\sum_{\alpha=1}^{n}\sum_{\beta=1}^{n}[\lambda_\alpha^{SK}(\mathbf{x}+\mathbf{h}) - \lambda_\alpha^{SK}(\mathbf{x})] \times[\lambda_\beta^{SK}(\mathbf{x}+\mathbf{h}) - \lambda_\beta^{SK}(\mathbf{x})]C(\mathbf{x}_\alpha - \mathbf{x}_\beta)\,\mathrm{d}\mathbf{x}. \quad (A.5)$$

In particular, it is seen that the conditional regional semi-variogram at lag $\mathbf{h}$ does not fluctuate around the prior semi-variogram model $\gamma(\mathbf{h})$. Its expected value depends on the domain on which it is computed, as well as the locations and values of the conditioning data (through the kriging weights and kriging predictions), and turns out to be unpractical to calculate.

Appendix B. Fluctuation covariance for the regional semi-variogram of a sum of independent and identically distributed random fields

Consider a set of independent stationary random fields $\{Y_j,\ j=1,\ldots,J\}$ with covariance function C and the same finite-dimensional distributions, and let us put

$$\forall \mathbf{x}\in R^d,\ Y^{(J)}(\mathbf{x}) = \frac{1}{\sqrt{J}}\sum_{j=1}^{J} Y_j(\mathbf{x}). \quad (B.1)$$

The random field $Y^{(J)}$ so defined has the same covariance function as each of the Y_j's. In the sequel, we will express the fluctuation covariance of its regional semi-variogram at lags $\mathbf{h}$ and $\mathbf{h}'$, denoted by $\Gamma_{D,J}(\mathbf{h})$ and $\Gamma_{D,J}(\mathbf{h}')$, respectively. To simplify the notations, let us introduce

$$\forall \mathbf{x}\in R^d,\ \forall j\in\{1,\ldots,J\},\ \Delta_j^{\mathbf{h}}(\mathbf{x}) = Y_j(\mathbf{x}+\mathbf{h}) - Y_j(\mathbf{x}). \quad (B.2)$$

Then

$$\mathrm{cov}[\Gamma_{D,J}(\mathbf{h}),\Gamma_{D,J}(\mathbf{h}')] = \frac{1}{J^2} \times\sum_{j,k,j',k'}\frac{\int_{D\cap D_{-\mathbf{h}}}\int_{D\cap D_{-\mathbf{h}'}}\mathrm{cov}[\Delta_j^{\mathbf{h}}(\mathbf{x})\Delta_k^{\mathbf{h}}(\mathbf{x}),\Delta_{j'}^{\mathbf{h}'}(\mathbf{x}')\Delta_{k'}^{\mathbf{h}'}(\mathbf{x}'))]\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'}{4K_{\mathbf{h}}(\mathbf{0})K_{\mathbf{h}'}(\mathbf{0})} \quad (B.3)$$

Since the Y_j's are independent random fields, the covariance terms are equal to zero, unless:

- $j=j'=k=k'$ (J terms), in which case one has

$$\frac{1}{J^2}\sum_{j=1}^{J}\frac{\int_{D\cap D_{-\mathbf{h}}}\int_{D\cap D_{-\mathbf{h}'}}\mathrm{cov}[\Delta_j^{\mathbf{h}}(\mathbf{x})^2,\Delta_j^{\mathbf{h}'}(\mathbf{x}')^2]\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'}{4K_{\mathbf{h}}(\mathbf{0})K_{\mathbf{h}'}(\mathbf{0})} = \frac{1}{J}\mathrm{cov}[\Gamma_{D,1}(\mathbf{h}),\Gamma_{D,1}(\mathbf{h}')], \quad (B.4)$$

- $j=j'\neq k=k'$, or $j=k'\neq j'=k$ ($2J^2-2J$ terms), in which case one has

$$\begin{aligned}&\mathrm{cov}[\Delta_j^{\mathbf{h}}(\mathbf{x})\Delta_k^{\mathbf{h}}(\mathbf{x}),\Delta_j^{\mathbf{h}'}(\mathbf{x}')\Delta_k^{\mathbf{h}'}(\mathbf{x}')]\\ &= \mathrm{cov}[\Delta_j^{\mathbf{h}}(\mathbf{x}),\Delta_j^{\mathbf{h}'}(\mathbf{x}')]\times\mathrm{cov}[\Delta_k^{\mathbf{h}}(\mathbf{x}),\Delta_k^{\mathbf{h}'}(\mathbf{x}')]\\ &= [C(\mathbf{x}+\mathbf{h}-\mathbf{x}'-\mathbf{h}') - C(\mathbf{x}-\mathbf{x}'-\mathbf{h}') - C(\mathbf{x}+\mathbf{h}-\mathbf{x}') + C(\mathbf{x}-\mathbf{x}')]^2. \end{aligned} \quad (B.5)$$

This is equal to half the covariance between the squared increments of a stationary Gaussian random field with covariance C (Eq. (11)). Accordingly,

$$\begin{aligned}&\frac{1}{J^2}\sum_{j\neq k}\frac{\int_{D\cap D_{-\mathbf{h}}}\int_{D\cap D_{-\mathbf{h}'}}\mathrm{cov}[\Delta_j^{\mathbf{h}}(\mathbf{x})\Delta_k^{\mathbf{h}}(\mathbf{x}),\Delta_j^{\mathbf{h}'}(\mathbf{x}')\Delta_k^{\mathbf{h}'}(\mathbf{x}')]\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'}{4K_{\mathbf{h}}(\mathbf{0})K_{\mathbf{h}'}(\mathbf{0})}\\ &= \frac{2J^2-2J}{J^2}\frac{1}{2}\mathrm{cov}[\Gamma_{D,\infty}(\mathbf{h}),\Gamma_{D,\infty}(\mathbf{h}')]\\ &= \left(1-\frac{1}{J}\right)\mathrm{cov}[\Gamma_{D,\infty}(\mathbf{h}),\Gamma_{D,\infty}(\mathbf{h}')], \end{aligned} \quad (B.6)$$

where $\Gamma_{D,\infty}$ is the regional semi-variogram of a Gaussian random field with covariance C (obtained asymptotically by letting J tend to infinity). By adding both contributions (B.4) and (B.6), one finally finds

$$\mathrm{cov}[\Gamma_{D,J}(\mathbf{h}),\Gamma_{D,J}(\mathbf{h}')] = \left(1-\frac{1}{J}\right)\mathrm{cov}[\Gamma_{D,\infty}(\mathbf{h}),\Gamma_{D,\infty}(\mathbf{h}')] + \frac{1}{J}\mathrm{cov}[\Gamma_{D,1}(\mathbf{h}),\Gamma_{D,1}(\mathbf{h}')]. \quad (B.7)$$

Appendix C. Supplementary materials

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.cageo.2007.12.012.

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