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REVISITING THE TURNING BANDS METHOD

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ABSTRACT

The problem of simulating a 3d stationary gaussian random function is considered. The turning bands method is a stereological device designed to reduce a 3d simulation into unidimensional ones. This paper mainly deals with the practical implementation of this method.

Keywords: gaussian random function, turning bands method, spectral method.

INTRODUCTION

A random function is said to be gaussian ("multigaussian" in the geostatistical jargon) if any linear combination of its variables follows a gaussian distribution. Its spatial distribution is totally characterized by its mean value m and its covariance function C.

This paper is devoted to the non-conditional simulation of stationary 3d gaussian random functions over a discrete or continuous three-dimensional domain D. In what follows, we shall assume $m = 0$ and $C(0) = 1$ (standard case).

An idea for a simulation algorithm is suggested by the Central Limit Theorem (Feller, 1971) which implies that under some mild assumptions the average of independent random functions (non necessarily gaussian) tends to become gaussian as their number becomes very large. To put this idea into practice, two questions must be considered:

i) How to generate random functions, not necessarily gaussian, with a given covariance function? In this paper, the turning bands method is investigated. Devised by Matheron in 1972, this method starts with the principle that it is easier to simulate along a line where the points are sequenced, rather than directly in $\mathbb{R}^3$. However, this method has met with resistance from practioners using simulations, mainly because of problem due to discretization and truncation. This paper sets out to show that these difficulties can be surmounted.

ii) How many random functions must be generated? To answer this question is not very

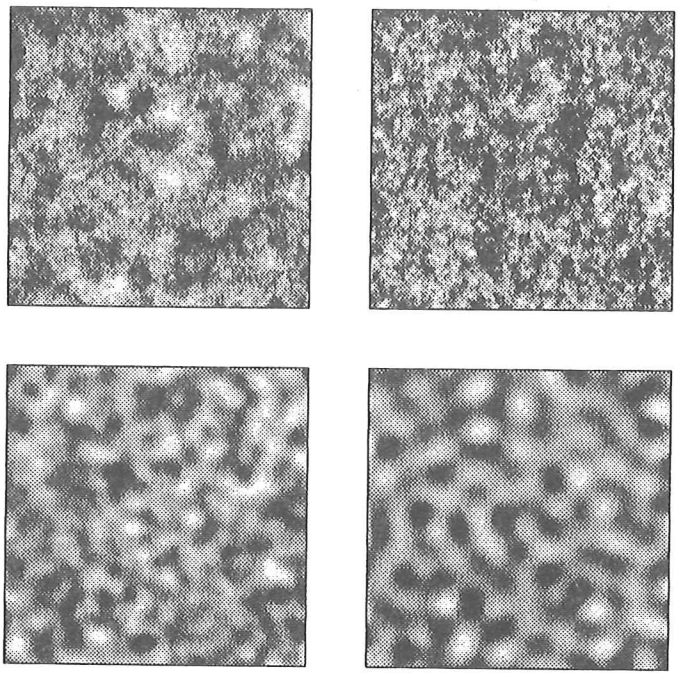

Figure 1. Some realizations of standard gaussian random functions with different covariance functions. From top to bottom and left to right, spherical, exponential, Gaussian and cardinal sine covariances.

easy because statistical deviations from the gaussian model can result either from a convergence problem (if the number of random functions is not large enough) or from a support problem (if the simulation domain is not large w.r.t. the covariance range). Both problems can be addressed by considering expansions related to the Central Limit Theorem, in particular the Berry-Esséen Theorem (Feller, 1971).

These two problems will be considered in turn.

THE TURNING BANDS METHOD

The covariance C is a positive definite function. If C is also continuous, Bochner's theorem states that it is the Fourier transform of a positive measure (the spectral measure), say χ

$$C(h) = \int_{\mathbb{R}^3} \exp\{i < u, h >\} \, d\chi(u) \tag{1}$$

Moreover, since $C(0) = 1$, χ is a probability distribution. Putting $u = (\theta, l)$ where θ is the direction of u (θ spans half a sphere, say S_2^+), and l is a location parameter ($-\infty < l < +\infty$), $d\chi(u)$ can be written as the product of the distribution $d\varpi(\theta)$ of θ by

the conditional distribution $d\varrho(l|\theta)$ of l given θ

$$d\chi(u) = d\varpi(\theta)\, d\varrho(l|\theta) \tag{2}$$

Replacing χ by its expression in formula (1) gives

$$C(h) = \int_{S_2^+} \int_{-\infty}^{+\infty} \exp\{il < \theta, h >\}\, d\varrho(l|\theta)\, d\varpi(\theta) \tag{3}$$

$$= \int_{S_2^+} C_\theta(< \theta, h >)\, d\varpi(\theta) \tag{4}$$

where C_θ is the unidimensional covariance

$$C_\theta(r) = \int_{-\infty}^{+\infty} \exp\{irl\}\, d\varrho(l|\theta) \tag{5}$$

The idea of the turning bands method is to reduce the simulation of a gaussian random function with covariance C to the simulations of independent stochastic processes with covariances C_θ. Let $(\theta_n, n \in I\!N)$ be a sequence of directions of S_2^+, and let $(X_n, n \in I\!N)$ be a sequence of independent stochastic processes with covariances C_{θ_n}. The random function

$$Y^{(n)}(x) = \frac{1}{\sqrt{n}} \sum_{k=1}^{n} X_k(< \theta_k, x >) \qquad x \in I\!R^3 \tag{6}$$

admits the covariance

$$C^{(n)}(h) = \frac{1}{n} \sum_{k=1}^{n} C_{\theta_k}(< \theta_k, h >) \tag{7}$$

As n becomes very large, the Central Limit Theorem implies that the spatial distribution of $Y^{(n)}$ tends to become gaussian with covariance $\lim_{n \longrightarrow +\infty} C^{(n)}$. This limit is exactly C in the case where $\frac{1}{n} \sum_{k=1}^{n} \delta_{\theta_k}$ converges weakly towards ϖ. The algorithm produced by the turning bands method is the following one:

i) generate a set of directions $\theta_1, ..., \theta_n$.
ii) generate independent standard stochastic process $X_1, ..., X_n$ with covariance functions $C_{\theta_1}, ..., C_{\theta_n}$.
iii) compute $\frac{1}{\sqrt{n}} \sum_{k=1}^{n} X_k(< \theta_k, x >)$ for any $x \in D$.

The calculation of the various covariances C_θ may not be always easy. However, in the particular case where the covariance C is isotropic, then ϖ is the Lebesgue measure over S_2^+ and all of the C_θ are equal to a same covariance function, say C_1. Its explicit value satisfies

$$C_1(r) = \frac{d}{dr}\Big(r\, C_3(r)\Big) \qquad r > 0 \tag{8}$$

where $C_3(|h|) = C(h)$ stands for the polar form of C.

Note also that the turning bands method tells nothing about the ways to generate the various directions θ_k or to simulate the stochastic processes X_k. This is the object of the next two sections.

SIMULATION OF THE STOCHASTIC PROCESSES

There exists many possible choices to simulate X_k, which makes the turning bands method very flexible. Consider, for instance, the case of an isotropic exponential covariance function

$$C(h) = \exp\{-|h|\} \qquad h \in I\!R^3 \tag{9}$$

The unidimensional covariance associated to the exponential covariance is

$$C_1(r) = (1 - |r|) \exp\{-|r|\} \qquad r \in I\!R \tag{10}$$

Three different methods are presented hereunder.

Let L be a random variable with p.d.f. $\frac{2}{\pi}\left(\frac{l}{1+l^2}\right)^2$, $l \in I\!R$ (the spectral density of C_1). Direct calculations show that if Φ is uniform over $(0, 2\pi)$, then the stochastic process

$$X_k(t) = \sqrt{2}\cos(Lt + \Phi) \qquad t \in I\!R \tag{11}$$

admits C_1 for its covariance function. This is exactly the formulation of the **spectral method** by Shinozuka (1972) among others. The spectral method has the potent advantage of being easily implementable (the spectral density can be simulated by acceptance-rejection), but the X_k's are not ergodic.

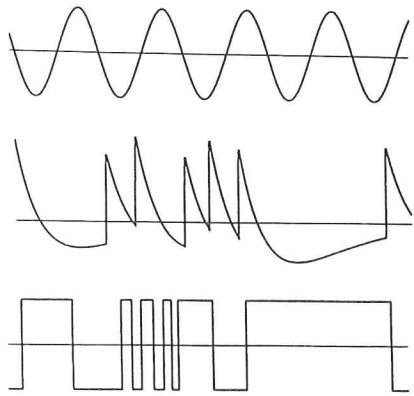

Figure 2. Simulation of an exponential covariance using the turning bands method. Three models for the unidimensional simulation. From top to bottom, the spectral method, the dilution method and the migration method.

To simulate the stochastic processes, one can also consider a **dilution process**, that is a moving average of functions located at random points. More formally

$$X_k(t) = \sum_{p \in \mathcal{P}} g(t - p) \tag{12}$$

where $\mathcal{P}$ is a Poisson point process in $I\!R$ of intensity 1, and g is the numerical function defined by

$$g(t) = (1 - t) \exp\{-t\}\, 1_{t \geq 0} \tag{13}$$

(Matheron, 1972; Journel, 1978), but this is not fully satisfactory as g does not have a bounded support.

A third possibility that has been inspired by **migration techniques** (Matheron, 1968) also exists:
i) generate a Poisson point process that partitions $\mathbb{R}$ into independent exponential intervals of mean length 2.
ii) split each interval into two halves, and set the first half to +1, the second half to −1.

Other algorithms for various types of covariances are given in (Lantuéjoul, 1994). In most cases, discretization and truncation problems can be avoided by using an appropriate simulation algorithm.

GENERATION OF THE DIRECTIONS IN THE ISOTROPIC CASE

In the isotropic case, ϖ is the Lebesgue measure over S_2^+ and can be approximated by a set of 15 regular directions at most (Journel and Huijbregts, 1978). To generate more directions, a possible approach is to compute an equidistributed sequence of points. A sequence of points is said to be **equidistributed** in S_2^+ if for any $B \subset S_2^+$, the proportion of points fallen within B from among the first n points tends to the ratio between the area of B and the one of S_2^+ as n becomes very large. For instance, a sequence of independent and uniform points in S_2^+ is equidistributed. But the crux is that there exist sequences that converge faster than independent and uniform points. Freulon (1992) suggested the following algorithm: he considers the binary and the ternary expansions of any integer $n = 1, 2, ...$

$$n = a_0 + 2a_1 + \cdots + 2^p a_p = b_0 + 3b_1 + \cdots + 3^q b_q \tag{14}$$

with $a_i = 0, 1$ and $b_j = 0, 1, 2$, from which 2 numbers between 0 and 1 are generated

$$u_n = \frac{a_0}{2} + \frac{a_1}{4} + \cdots + \frac{a_p}{2^{p+1}} \qquad v_n = \frac{b_0}{3} + \frac{b_1}{9} + \cdots + \frac{b_q}{3^{q+1}} \tag{15}$$

The coordinates of the n^{th} point of the sequence are

$$\theta_n = \left(\cos(2\pi u_n)\sqrt{1-v_n^2}\ ,\ \sin(2\pi u_n)\sqrt{1-v_n^2}\ ,\ v_n\right) \tag{16}$$

Figure 3 shows a comparison of 400 independent and uniform points with the 400 points generated according the previous algorithm.

In the case where the θ_k's have been independently and uniformly generated, it is possible to assess how the spatial distribution of

$$Y^{(n)}(x) = \frac{1}{\sqrt{n}} \sum_{k=1}^{n} X_k(< \theta_k, x >) \qquad x \in \mathbb{R}^3 \tag{17}$$

departs from a gaussian distribution, or equivalently, if $x_1, ..., x_p$ stand for any set of points, and if $\lambda_1, ...\lambda_p$ denote any set of numbers, how does the distribution of $\sum_{j=1}^{p} \lambda_j Y^{(n)}(x_j)$ departs from a gaussian distribution with mean 0 and variance $\sigma^2 = \sum_{j,j'=1,p}^{p} \lambda_j \lambda_{j'} C(x_j - x_{j'})$? Provided that the distribution of $\sum_{j=1}^{p} \lambda_j X_k(< \theta_k, x_j >)$ admits an finite third order absolute moment, say μ_3, a possible answer is given by the Berry-Esséen theorem (Feller,

1971). This theorem gives an upper bound for the difference between the standardized distribution of the average, and the standard gaussian distribution G

$$\sup_{u \in \mathbb{R}} \left| P\left\{ \frac{\sum_{j=1}^{p} \lambda_j Y^{(n)}(x_j)}{\sigma} < u \right\} - G(u) \right| < \frac{\alpha}{\sqrt{n}} \frac{\mu_3}{\sigma^3} \tag{18}$$

where α is a numerical constant less than 1.32132. A more restrictive approach consists of comparing the moments of $Y^{(n)}$ with those of a standard gaussian random function (Lantuéjoul, 1994). The two-dimensional case of a regular set of directions has been studied by Mantoglou and Wilson (1982). General results related to the case of an equidistributed sequence of points are not known so far.

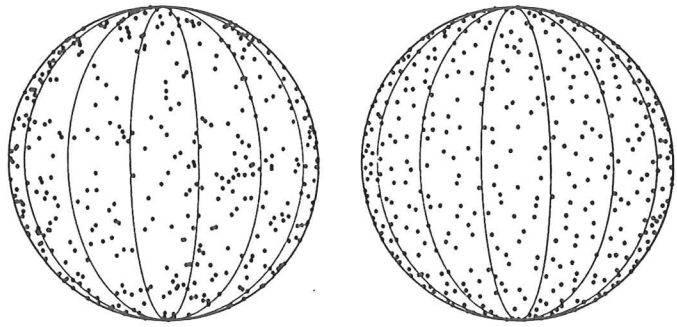

Figure 3. Generation of 400 points on the unit sphere. On the left, the points are independent and uniform. On the right, they are located according to an equidistributed sequence.

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