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# THE GENERALIZED VARIOGRAM

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**Abstract.** Although stationary phenomena are characterized by their covariance, the structural tool is the variogram. In the case of nonstationary phenomena, the variogram is not experimentally accessible, so that blind methods are often used for the identification of the ordinary or generalized covariance. However, if regularly spaced data are available (at grid nodes or along profiles), the generalized variogram can be computed. It filters any polynomial trend up to a given degree. Its relation with the covariance is nearly as simple as for the ordinary variogram. The theory of the generalized variogram is presented: definition, relation with the ordinary or generalized covariance, estimation and fluctuations in the Gaussian and non-Gaussian cases.

**Key words:** Covariance, generalized covariance, variogram, variogram of residuals, generalized variogram, intrinsic random function, drift, trend.

## INTRODUCTION

Although stationary phenomena are characterized by their covariance function, the advantage of the variogram as a structural tool is well known (Jowett, 1955; Matheron, 1965). But when dealing with strongly nonstationary phenomena, we must resort to inference methods that give rise to bias problems (e.g., variogram of residuals; cf. Matheron, 1970; Sabourin, 1976) or to more-or-less blind methods (automatic fitting of the coefficients of a polynomial generalized covariance; cf. Delfiner, 1976). If regularly spaced data are available (e.g., at grid nodes, or along profiles, which is more and more common in surveys with continuous measurements), the generalized variogram, which has been presented and applied to actual data by Chilès (1979) and Chilès and Gable (1984), can be used profitably. Published papers show a constant interest in nonstationary models and their inference: Starks and Fang (1982), Kitanidis (1983, 1985), Marshall and Mardia (1985), Stein (1986), Campbell (1988), Zimmerman (1989), Dimitrakopoulos (1990), Pardo Igúzquiza and Dowd (2003), Bosch et al. (2009), etc. In the case of regularly spaced data, Cressie (1987) has proposed a tool which is similar to the generalized variogram, but more difficult to interpret. Chauvet (1987) has investigated the use of the covariance of generalized increments, a tool which is very powerful, but requires more care in its interpretation. This paper presents the generalized variogram theory in a comprehensive manner: definition, relation with the ordinary or generalized covariance, estimation and modeling in Gaussian and non-Gaussian cases.

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<sup>1</sup> This technical note, written in 2012, is based on a previous note in French (Chilès, 1979), supplemented in 1989 by numerical calculations of estimation and fluctuation variances of the generalized variogram. An expanded summary is included in Chapter 4 of Chilès and Delfiner (1999).

## RECALL ON RANDOM FUNCTION MODELS

Only a brief recall will be presented. Comprehensive presentations can be found in Matheron (1970, 1973), Cressie (1987), and Chilès and Delfiner (1999).

### Regionalized Variable—Random Function

Let  $z(x)$  be a regionalized variable, that is, a function of point  $x \in D$ , where  $D$  is a subset of the Euclidean space  $\mathbb{R}^n$  (usually  $n \leq 3$ ). Because of its double—simultaneously random and structured—character, this regionalized variable is considered as a realization of a random function (RF)  $Z(x)$ . It is also assumed that  $z(x)$  is the unique known realization of  $Z(x)$ , which is usually the case in earth science applications. No inference of the random function is then possible, unless complementary assumptions of ergodicity and stationarity are introduced that allow the replacement of averages on all possible realizations by spatial averages on a single realization. As a single realization is considered, the choice of a model which would not satisfy the ergodicity hypothesis would have no objective meaning (Matheron, 1978, pp. 103-106). So, without loss of generality, ergodic models will be considered. Concerning stationarity, a too strict assumption can be inconsistent with the data. Several models have been developed, with the aim of weakening the necessary stationarity assumptions. Because only the first two moments of the random function—and not its whole spatial distribution—will be used, some kind of second-order stationarity will be assumed.

### Stationary Random Function (SRF)

The simplest model is that of (second-order) stationary random functions (SRF). The mathematical expectation of  $Z(x)$  is equal to a constant  $m$  that we assume known and that we take equal to zero—without loss of generality—and the covariance between  $Z(x)$  and  $Z(x + h)$  is a function of the separation vector  $h$  only:

$$E[Z(x)] = 0$$

$$E[Z(x) Z(x + h)] = C(h)$$

The covariance  $C(h)$  is a positive definite function, which warrants that the variance  $\int \int \lambda(dx) C(x' - x) \lambda(dx')$  of any linear combination  $\int \lambda(dx) Z(x)$  is positive or null. Here the measure  $\lambda$  is a combination of Dirac measures, so that the integral  $\int \lambda(dx) Z(x)$  is a finite sum, assigning weights  $\lambda_i$  to points  $x_i$ . This property applies also to linear functionals but these will not be considered here.

### Universal Kriging Model (UK)

In many applications, the stationary character fails because of the presence of a trend. This led Matheron (1969) to define a less restrictive model, the universal kriging (UK) model, where  $Z(x)$  is the sum of two terms:

$$Z(x) = m(x) + Y(x)$$

where:

- The drift  $m(x) = E[Z(x)]$  is a function that varies slowly and that locally admits a representation of the form

$$m(x) = \sum_{\ell=0}^L a_{\ell} f^{\ell}(x),$$

where the  $f^{\ell}$  functions are all the monomials of degree  $\leq k$  (degree of the drift) and the  $a_{\ell}$ 's are unknown coefficients. The total number of monomials, denoted  $L + 1$ , is equal to  $k + 1$  in  $\mathbb{R}^1$ ,  $(k + 1)(k + 2) / 2$  in  $\mathbb{R}^2$ ,  $(k + 1)(k + 2)(k + 3) / 6$  in  $\mathbb{R}^3$ , and  $\binom{k+n}{k}$  in  $\mathbb{R}^n$ .

- The random component  $Y(x)$  is a zero-mean SRF with covariance  $C(h)$ .

If  $k = 0$ , the drift  $m(x)$  is reduced to the constant term  $a_0$  and the model locally corresponds to an SRF with an unknown mean. It is also possible to define a UK model with  $f^{\ell}$  functions other than monomials, but such a model will not be considered.

### Admissible Linear Combinations (ALC- $k$ )—Generalized Increments (GI- $k$ )

Within the framework of the UK model, the shape of the drift—that is, its degree  $k$ —is assumed to be known, but the  $a_{\ell}$  coefficients are unknown. For the computation of second-order moments of  $Z(x)$ , it is therefore necessary to only use linear combinations (or more generally linear functionals) that are independent of the  $a_{\ell}$ 's—that is, that filter the drift whatever the  $a_{\ell}$ 's. More explicitly, this means that we will only consider the variance of linear combinations  $Z(\lambda) = \int \lambda(dx) Z(x)$  that satisfy

$$\int \lambda(dx) f^{\ell}(x) = 0 \quad \ell = 0, 1, \dots, L \quad (1)$$

(i.e., for any monomial of degree  $\leq k$ ). We recall that  $\lambda$  is a combination of Dirac measures, so that these integrals are finite sums.

A linear combination satisfying (1) is called an *allowable linear combination of order  $k$*  (ALC- $k$ ); it is also called *authorized linear combination of order  $k$* , or *generalized increment of order  $k$*  (GI- $k$ ).

Note that conditions (1) are a generalization of the universality conditions of UK: Indeed, when  $Z(x_0)$  is estimated at an unsampled point  $x_0$  by some linear combination  $\sum_{i=1}^N \lambda_i Z(x_i)$  of the  $N$  data values, the universality conditions

$$\sum_{i=1}^N \lambda_i f^{\ell}(x_i) = f^{\ell}(x_0), \quad \ell = 0, 1, \dots, L$$

are imposed to ensure an unbiased estimation whatever the  $a_\ell$ 's. The estimation error is  $\sum_{i=1}^N \lambda_i Z(x_i) - Z(x_0)$ . It is of the form  $\int \lambda(dx) Z(x)$ , where  $\lambda$  is the linear combination with weight  $\lambda_i$  at point  $x_i$  and  $\lambda_0 = -1$  at point  $x_0$  and satisfies (1).

### **Intrinsic Random Functions (IRF- $k$ )**

Instead of focusing the attention on the function  $Z(x)$  itself, the theory of intrinsic random functions (Matheron, 1971, 1973) lays stress on generalized increments:

By definition,  $Z(x)$  is an intrinsic random function of order  $k$  (IRF- $k$ ) if and only if for any ALC- $k$   $\lambda$  the random function  $Z_\lambda(x) = \int \lambda(du) Z(x+u)$  is a zero-mean SRF.

### **Generalized Covariance (GC)**

The covariance function of an SRF is a positive definite function, because this is the condition for the variance of any linear combination to be non-negative. If only ALC- $k$  are taken, there is no need to be so exacting, and one can consider as a generalized covariance any function  $K(h)$  such that  $\int \int \lambda(dx) K(x'-x) \lambda(dx')$  is non-negative for any ALC- $k$   $Z(\lambda)$ . From this point of view, the main property of an IRF- $k$  is as follows (Matheron, 1973, p. 450, as a consequence of Gel'fand-Vilenkin theory):

- i) If  $Z(x)$  is an IRF- $k$ , there exists a generalized covariance  $K(h)$  such that the covariance of any pair of ALC- $k$   $Z(\lambda)$  and  $Z(\mu)$  is of the form

$$\text{Cov}(Z(\lambda), Z(\mu)) = \int \int \lambda(dx) K(x'-x) \mu(dx').$$

- ii) This generalized covariance is unique up to an even polynomial of degree  $2k$  (if an even polynomial of degree  $\leq 2k$  is added, then  $\int \int \lambda(dx) K(x'-x) \mu(dx')$  remains unchanged when  $Z(\lambda), Z(\mu)$  are ALC- $k$ ).

A well-known particular case is  $k=0$ , which corresponds to the ordinary intrinsic random functions: Only linear combinations satisfying  $\int \lambda(dx) = 0$  are used for variance and covariance computations. The GC is defined up to a constant; the GC  $K(h)$  such that  $K(0) = 0$  is equal to  $-\gamma(h)$ , where  $\gamma(h)$  is the variogram  $\frac{1}{2}\text{Var}[Z(x+h) - Z(x)]$ .

### **Generalized Covariance Models**

Except in the stationary case (which can be seen as the case where  $k=-1$ ), the GC  $K(h)$  is not the covariance of  $Z(x)$  and  $Z(x+h)$ , which may not be defined. The GC can be used only for calculating variances and covariances of ALC- $k$ . When the value of the order  $k$  increases, the class of the ALC- $k$  shrinks, and conversely the class of the GC functions expands (hence the class of phenomena that can be modeled by such random functions expands).

In practice, the basic generalized covariance models used at order  $k$  are:

- the ordinary covariance functions of SRFs.
- the *power law model*

$$(-1)^{1+\lfloor \alpha/2 \rfloor} |h|^\alpha, \quad 0 < \alpha < 2k + 2, \quad \alpha \text{ not even}$$

where  $\lfloor \cdot \rfloor$  is the floor function—that is,  $\lfloor u \rfloor$  is the largest integer not greater than  $u$ .  $(-1)^{1+\lfloor \alpha/2 \rfloor}$  thus gives the sign of the covariance. This sign alternates with the value of  $\alpha$ : It is negative for  $0 < \alpha < 2$ , positive for  $2 < \alpha < 4$ , negative for  $4 < \alpha < 6$ , and so on (Matheron, 1973, p. 452). Note that we do not take even values of  $\alpha$ , as a GC is defined up to an even polynomial of degree  $2k$ .

- the generalized covariance

$$(-1)^{m+1} |h|^{2m} \log |h|, \quad 1 \leq m \leq k$$

which is obtained as the limit of  $(-1)^{m+1} [|h|^{2m+\varepsilon} - |h|^{2m}] / \varepsilon$  when  $\varepsilon > 0$  tends to 0 (Chauvet 1987, pp. 53–54; Chilès and Delfiner, 1999, p. 264, or 2012, p. 266). In  $\mathbb{R}^2$  the covariance  $|h|^2 \log |h|$  with  $k = 1$  is of particular interest, because in this case kriging coincides with spline interpolation (Matheron, 1980, 1981; Dubrule, 1983).

- the *polynomial generalized covariance*

$$\sum_{m=0}^k (-1)^{m+1} b_{2m+1} |h|^{2m+1}$$

where the  $b_{2m+1}$  coefficients satisfy some suitable restrictions (Matheron, 1973, p. 452; a sufficient condition is  $b_{2m+1} \geq 0$  for every  $m$ ). If we add a nugget effect component  $C_0 \delta(h)$ , where  $\delta$  is the Dirac delta function, and logarithmic terms, we get the more general *polynomial/logarithmic model*

$$K(h) = C_0 \delta(h) + \sum_{m=0}^k (-1)^{m+1} b_{2m+1} |h|^{2m+1} + \sum_{m=1}^k (-1)^{m+1} b_{2m} |h|^{2m} \log |h| \quad (2)$$

with  $C_0 \geq 0$ ,  $b_{2m+1} \geq 0$ ,  $b_{2m} \geq 0$  for every  $m$  (as previously stated this is a sufficient condition). Note that these models do not include even monomials, because  $K(h)$  is defined up to an even polynomial of degree  $\leq 2k$ , which would contribute for 0 in the variance of an ALC- $k$ .

## IDENTIFICATION OF THE GENERALIZED COVARIANCE: THE GENERALIZED VARIOGRAM

### The Problem

Once the degree  $k$  and the GC  $K(h)$  are known, estimation by kriging can be easily performed (Matheron, 1973, pp. 457–460). The key problem is in fact the determination of the GC. Because  $K(h)$  is not the covariance of  $Z(x)$  and  $Z(x+h)$ , it cannot be determined for a given  $h$

by taking pairs of points a distance  $h$  apart, as is done for the ordinary covariance of a zero mean SRF. In the general case of scattered data, an automatic fitting to a model of the type

$$K(h) = \sum_m b_m K_m(h)$$

is usually performed, where the  $K_m$ 's are a priori given elementary GC models and the  $b_m$ 's are the coefficients to be fitted (see Delfiner, 1976; Chilès, 1978; Kitanidis, 1985; Marshall and Mardia, 1985; Stein, 1986; Chilès and Delfiner, 1999). The a priori model, usually a polynomial GC with a nugget effect, can be ill-adapted. Therefore a non-parametric evaluation of the GC would be useful.

Apart from the stationary case with zero mean, which is practically never encountered and for which the GC  $K(h)$  coincides with the ordinary covariance  $C(h)$ , there exists an important case where  $K(h)$  can be inferred by means of a non-parametric method. This is the case of the ordinary IRF, or IRF-0. The usual structural tool is the variogram

$$\gamma(h) = \frac{1}{2} \text{Var}[Z(x+h) - Z(x)]$$

which is linked with the GC by the relation

$$\gamma(h) = K(0) - K(h)$$

As the GC is defined up to a constant, it can be taken as  $-\gamma(h)$ .

The variogram is based on the variance of the increment  $Z(x+h) - Z(x)$ , which is the simplest ALC-0. The obvious generalization when  $k > 0$  is to use the variance of the finite difference of order  $k + 1$ .

### Finite Differences of Order $k + 1$

The generalization of the simple increment or finite forward difference

$$\Delta_h Z(x) = Z(x+h) - Z(x)$$

is the increment or finite forward difference of order  $k + 1$ , which is the simplest ALC- $k$  in 1D:

$$\begin{aligned} \Delta_h^{k+1} Z(x) &= \sum_{q=0}^{k+1} (-1)^q \binom{k+1}{q} Z(x + (k+1-q)h) \\ &= (-1)^{k+1} \sum_{p=0}^{k+1} (-1)^p \binom{k+1}{p} Z(x + ph) \end{aligned} \quad (3)$$

The increments of successive orders are linked by the recurrence relationship

$$\Delta_h^{k+1} Z(x) = \Delta_h (\Delta_h^k Z(x))$$



The computation of finite differences of successive orders is commonly used in the study of nonstationary time series, in order to get roughly stationary variables (ARIMA models; see Box and Jenkins, 1970). Indeed, just as the simple increment filters any constant term, the increment of order  $k + 1$  filters any polynomial component of degree  $\leq k$ . Other 1D ALC- $k$  could be considered (e.g., the one used by Cressie, 1987).

An interesting property has been demonstrated by Chauvet (1987, pp. 29–31): Any 1D ALC- $k$  built on regularly spaced points can be decomposed into a sum of increments of order  $k + 1$  with  $h$  equal to the spacing, and the decomposition is unique.

### Generalized Variogram of Order $k$ (GV)

By definition, the generalized variogram of order  $k$ , denoted by  $\Gamma(h)$  and abbreviated as GV, is the appropriately scaled variance of the increment of order  $k + 1$ :

$$\Gamma(h) = \frac{1}{M_k} \text{Var} \left[ \Delta_h^{k+1} Z(x) \right] \quad (4)$$

The scaling factor  $M_k = \binom{2k+2}{k+1}$  is introduced to ensure that, in case of a pure nugget effect  $C_0$ , we have

$$\Gamma(h) = \begin{cases} 0 & \text{if } h = 0 \\ C_0 & \text{if } h \neq 0 \end{cases}$$

as for an ordinary variogram.

Here we find a justification for naming  $\gamma(h)$  a variogram rather than a *semi*-variogram; otherwise  $\Gamma(h)$  would not be the generalized variogram, even less the generalized semi-variogram, but the  $M_k$ th of a generalized variogram! Actually, if the term semi-variogram has been used in the first geostatistical publications (Matheron, 1965), the term variogram has been previously defined by Jowett (1955) as the experimental graph of  $\gamma(h)$ .

Explicitly we have:

$$\begin{cases} k = 1: & \Gamma(h) = \frac{1}{6} \text{Var} [Z(x + 2h) - 2 Z(x + h) + Z(x)] \\ k = 2: & \Gamma(h) = \frac{1}{20} \text{Var} [Z(x + 3h) - 3 Z(x + 2h) + 3 Z(x + h) - Z(x)] \\ k = 3: & \Gamma(h) = \frac{1}{70} \text{Var} [Z(x + 4h) - 4 Z(x + 3h) + 6 Z(x + 2h) - 4 Z(x + h) + Z(x)] \end{cases}$$

The first definition of the generalized variogram can be found in Matheron (1972, p. 3). It was first used by Orfeuill (1972), who computed the sample GVs of simulations of IRF- $k$  with given GC  $K(h)$  in order to compare them with their theoretical value. This is a function of the GC, as it will be seen now.

## Relationship Between Generalized Variogram and Generalized Covariance

Because the increment of order  $k + 1$  is an ALC- $k$ , its variance can be expressed in terms of the generalized covariance. Applying the definition of a generalized covariance to (4) gives

$$\Gamma(h) = \frac{1}{M_k} \sum_{p=-k-1}^{k+1} (-1)^p \binom{2k+2}{k+1+p} K(ph) \quad (5)$$

Explicitly

$$\begin{cases} k = 1: & \Gamma(h) = K(0) - \frac{4}{3} K(h) + \frac{1}{3} K(2h) \\ k = 2: & \Gamma(h) = K(0) - \frac{3}{2} K(h) + \frac{3}{5} K(2h) - \frac{1}{10} K(3h) \\ k = 3: & \Gamma(h) = K(0) - \frac{8}{5} K(h) + \frac{4}{5} K(2h) - \frac{8}{35} K(3h) + \frac{1}{35} K(4h) \end{cases}$$

While being simple, the relationship between  $\Gamma$  and  $K$  is more complex than in the case of an ordinary variogram. In particular, whether the GV determines the GC (up to the even polynomial) is still an unsolved problem. Chauvet (1987) has studied this problem in the 1D case in a more general framework: Since  $\Delta_h^{k+1} Z(x)$  is an SRF, its covariance can be defined as

$$C_h(l) = E \left[ \Delta_h^{k+1} Z(x) \Delta_h^{k+1} Z(x+l) \right] \quad (6)$$

The generalized variogram  $\Gamma(h)$  is equal to  $\frac{1}{M_k} C_h(0)$ . The covariance  $C_h(l)$  is obviously a more powerful tool than the generalized variogram, but its interpretation is also more complex. From definitions (3) and (6), it is linked with the GC through the relation (e.g., Chauvet, 1987, p. 41):

$$C_h(l) = \sum_{p=-k-1}^{k+1} (-1)^p \binom{2k+2}{k+1+p} K(l+ph) \quad (7)$$

Chauvet (1987, pp. 108–111) has proven that the knowledge of  $C_h(l)$  for any  $h$  and  $l$  determines the GC  $K(h)$  (up to the minimum indetermination). But it is not so obvious whether the knowledge of the sole GV  $\Gamma(h)$  (i.e., of  $C_h(l)$  for any  $h$ , but only for  $l=0$ ) characterizes the GC. Expressed in its generality, the problem has not been solved up to now (Chauvet, 1987, pp. 215–231).

However, there are two important cases where the GV does determine the GC (up to the even polynomial): (i) when the GC is bounded (the GC amounts to an ordinary covariance), and (ii) when the GC is a sum of power law models, and in particular when it is a polynomial/logarithmic generalized covariance.

*Case of the power law model*

If  $K(h)$  behaves like  $|h|^\alpha$ , or more generally if it is a sum of power-law models of the form

$$K(h) = \sum_{\alpha} (-1)^{1+\lfloor \alpha/2 \rfloor} b_{\alpha} |h|^{\alpha}$$

with non-even powers  $\alpha$  comprised between 0 and  $2k+2$  and positive coefficients  $b_{\alpha}$ , then  $\Gamma(h)$  has the same form: According to (5), only the coefficients change:

$$\Gamma(h) = \sum_{\alpha} (-1)^{1+\lfloor \alpha/2 \rfloor} b_{\alpha} B_{\alpha} |h|^{\alpha}$$

with

$$B_{\alpha} = \frac{1}{M_k} \sum_{p=-k-1}^{k+1} (-1)^p \binom{2k+2}{k+1+p} |p|^{\alpha} \quad (8)$$

In particular, a polynomial GC leads to a polynomial GV.

Even values for  $\alpha$  are excluded from the power law model—they would give a zero contribution to the GV. Conversely, a GC of the form  $K(h) = (-1)^{m+1} b_{2m} |h|^{2m} \log |h|$ , with  $1 \leq m \leq k$ , leads to the even GV  $\Gamma(h) = (-1)^{m+1} b_{2m} B_{2m} |h|^{2m}$  with

$$B_{2m} = \frac{1}{M_k} \sum_{p=-k-1}^{k+1} (-1)^p \binom{2k+2}{k+1+p} |p|^{2m} \log(|p|)$$

(with the convention that the term corresponding to  $p=0$  in this sum is zero). Consequently, if the GC  $K(h)$  follows a polynomial/logarithmic model (2), the GV  $\Gamma(h)$  is a polynomial of degree  $2k+1$  in  $|h|$ , where all the logarithmic terms of  $K(h)$  have turned into even degree terms. Explicit results are given below (where  $h$  stands for  $|h|$ ):

$$k=1 \begin{cases} K(h) = C_0 \delta(h) - b_1 h + b_2 h^2 \log h + b_3 h^3 \\ \Gamma(h) = C_0 [1 - \delta(h)] + \frac{2}{3} b_1 h + \frac{4}{3} \log 2 b_2 h^2 + \frac{4}{3} b_3 h^3 \end{cases}$$

$$k=2 \begin{cases} K(h) = C_0 \delta(h) - b_1 h + b_2 h^2 \log h + b_3 h^3 - b_4 h^4 \log h - b_5 h^5 \\ \Gamma(h) = C_0 [1 - \delta(h)] + \frac{3}{5} b_1 h + \frac{3}{10} (8 \log 2 - 3 \log 3) b_2 h^2 + \frac{3}{5} b_3 h^3 \\ \quad + \frac{3}{10} (27 \log 3 - 32 \log 2) b_4 h^4 + \frac{33}{5} b_5 h^5 \end{cases}$$

$$k=3 \begin{cases} K(h) = C_0 \delta(h) - b_1 h + b_2 h^2 \log h + b_3 h^3 - b_4 h^4 \log h - b_5 h^5 + b_6 h^6 \log h + b_7 h^7 \\ \Gamma(h) = C_0 [1 - \delta(h)] + \frac{4}{7} b_1 h + \frac{72}{35} (2 \log 2 - \log 3) b_2 h^2 + \frac{16}{35} b_3 h^3 \\ \quad + \frac{24}{35} (27 \log 3 - 40 \log 2) b_4 h^4 + \frac{16}{7} b_5 h^5 \\ \quad + \frac{8}{35} (1248 \log 2 - 729 \log 3) b_6 h^6 + \frac{2416}{35} b_7 h^7 \end{cases}$$

### *Case of an ordinary covariance*

If  $K(h)$  is an ordinary covariance with range  $a$  and value  $C$  at  $h = 0$ , then  $\Gamma(h) = C$  for  $|h| \geq a$ . In other words,  $\Gamma(h)$  has the same range and sill as the ordinary variogram  $K(0) - K(h)$ . Consequently, the nugget effect, if any, remains the same. The behavior near the origin is polynomial in all common covariance models, and hence remains polynomial, but with changes in the coefficients; in particular, the even terms of degree  $\leq 2k$  disappear. Figure 1 displays the GVs associated with the spherical, cubic, exponential, and Gaussian covariances, where these models are defined as:

- Spherical model:

$$K(h) = \begin{cases} C\left(1 - \frac{3}{2}r + \frac{1}{2}r^3\right) & \text{if } r \leq 1 \\ 0 & \text{if } r \geq 1 \end{cases} \quad \text{with } r = |h|/a$$

- Cubic model:

$$K(h) = \begin{cases} C\left(1 - 7r^2 + \frac{35}{4}r^3 - \frac{7}{2}r^5 + \frac{3}{4}r^7\right) & \text{if } r \leq 1 \\ 0 & \text{if } r \geq 1 \end{cases} \quad \text{with } r = |h|/a$$

- Exponential model:

$$K(h) = C \exp(-|h|/a)$$

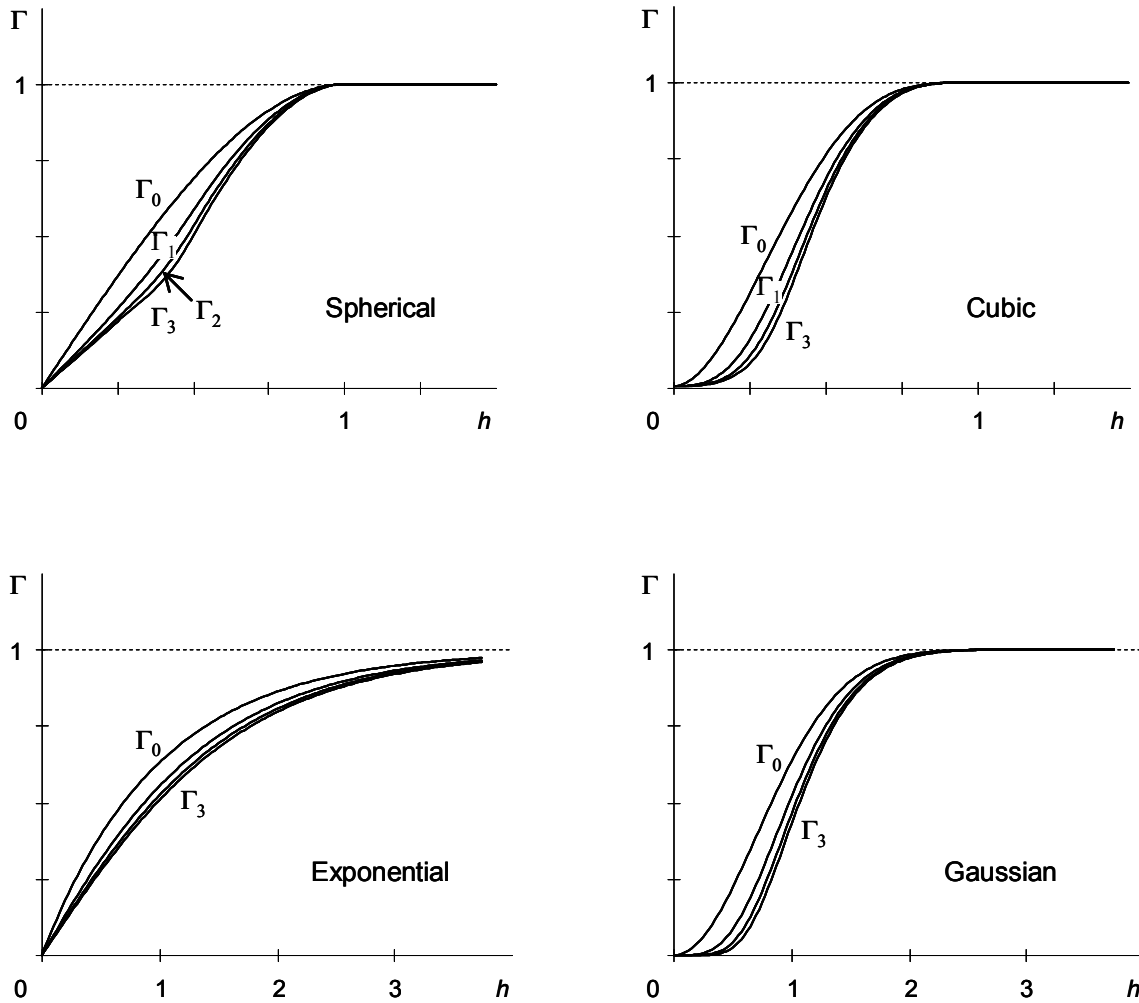
- Gaussian model:

$$K(h) = C \exp(-|h|^2/a^2)$$

### **Variogram Fitting**

From a practical viewpoint, it should be kept in mind that the objective is to identify the GC function  $K(h)$ , since it is the one involved in estimation problems. So, after computing a sample GV, one will try to fit a linear combination of GV models associated with given GC models. As the GV models remain close to the GC models, fitting a sample GV is not more difficult than fitting an ordinary sample variogram. In particular, automatic fitting procedures of sample variograms like that proposed by Desassis and Renard (2012) can be easily adapted to fit sample GVs. (The procedure of these authors is iterative and fits the ranges and sills of the various components.) In the special case of a polynomial/logarithmic GC, the situation is very simple: The coefficients of the GC model derive directly from the fitting of a polynomial with positive coefficients to the sample GV.

The validity of the method can be examined from the point of view of sampling theory. But let us first present a case study.

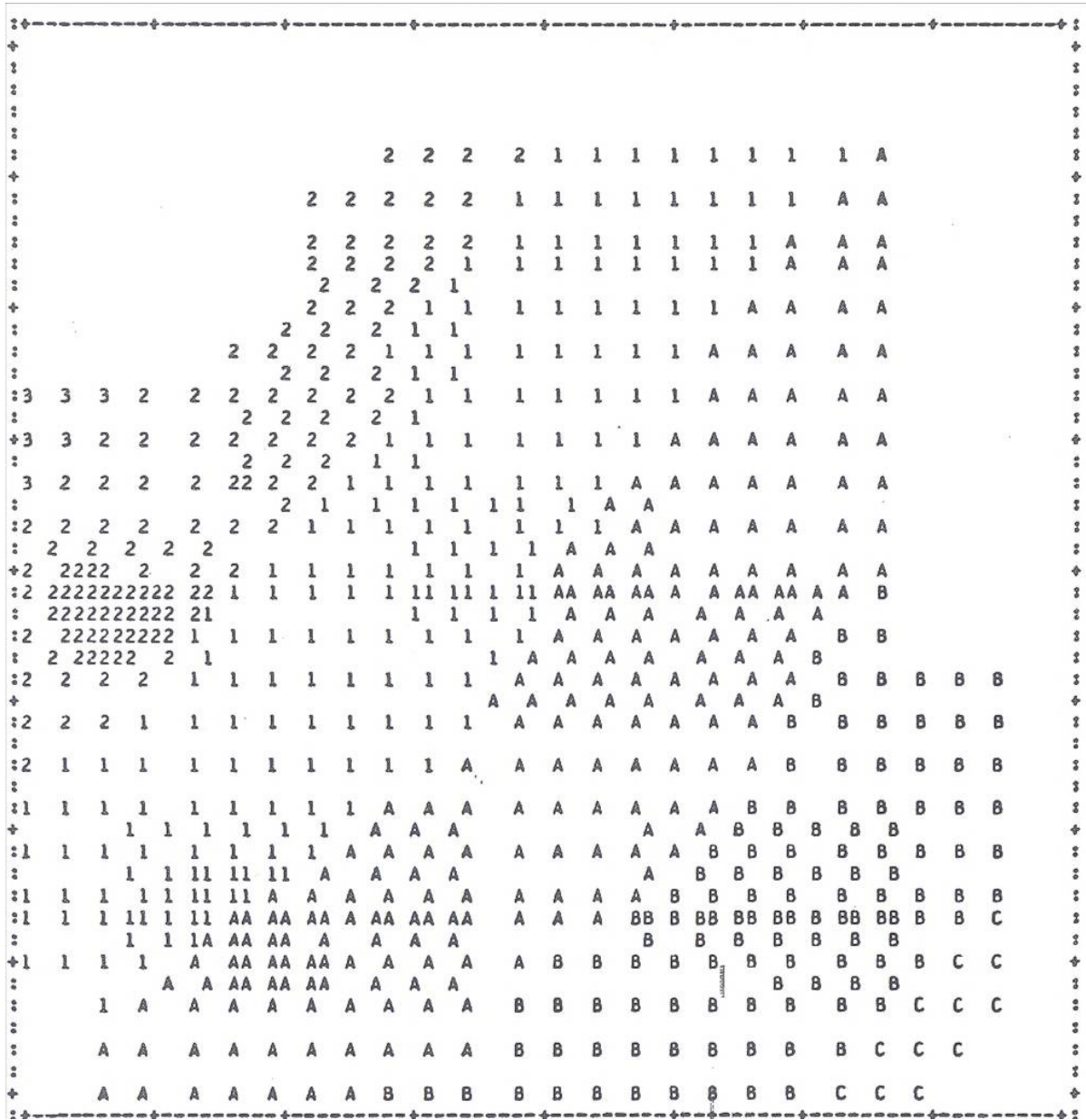


**FIGURE 1.** Generalized variograms  $\Gamma_k$  associated with four classical covariance models (spherical, cubic, exponential, and Gaussian covariances) for  $k = 0, 1, 2, 3$ .

## A CASE STUDY

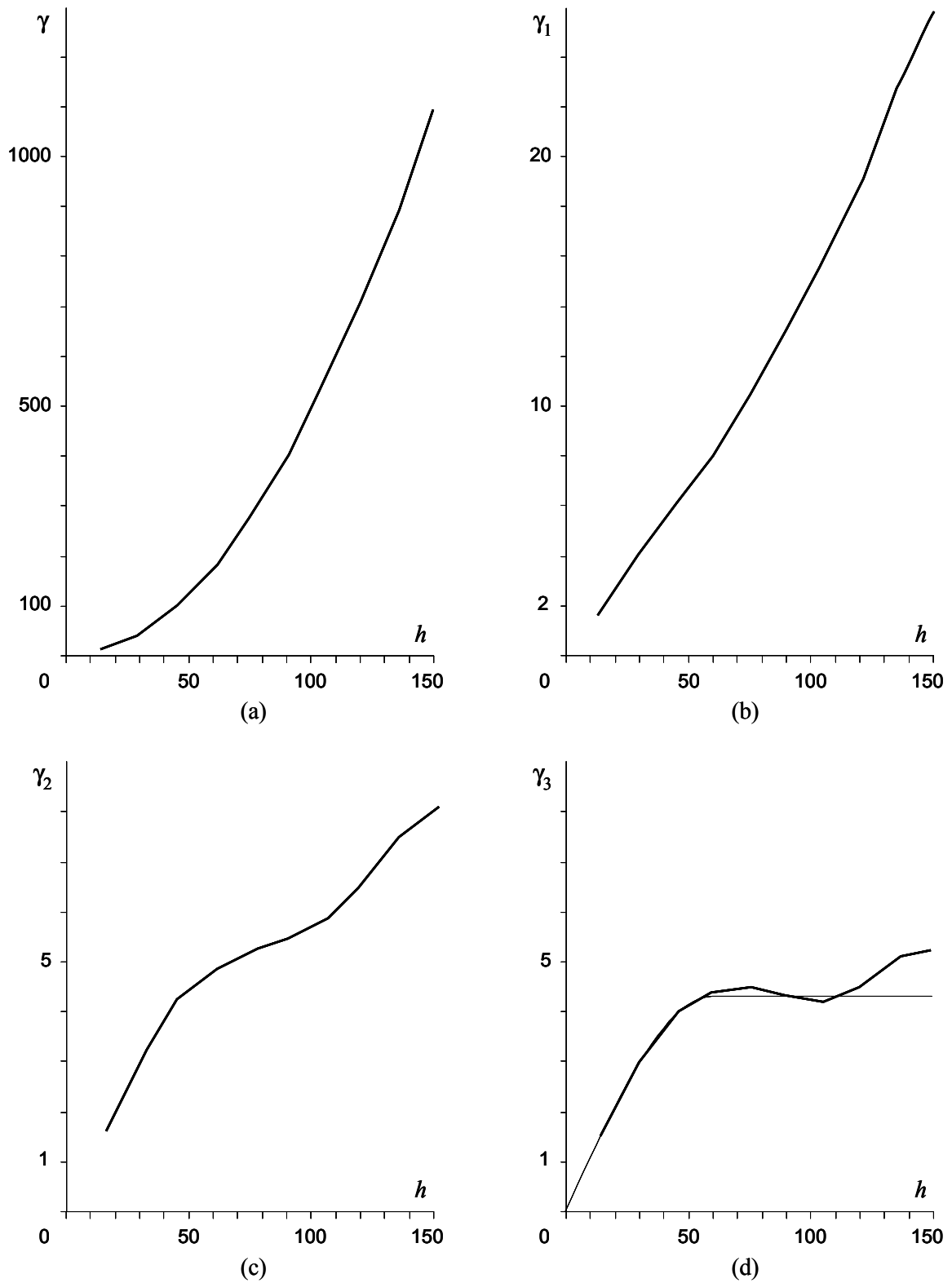
We consider civil-engineering microgravimetric data (Bouguer anomaly, quarry of Ariana, Tunisia). These data comprise 502 points on a 15-m grid, supplemented by 250 points where anomalies are suspected. The measurements were done with an accuracy of  $\pm 4 \mu\text{gal}$ . Assuming that this accuracy corresponds to twice the standard deviation of a Gaussian error, the measurement error variance is  $C_0 = 4 \mu\text{gal}^2$ . This is the value we will use, because the variograms will show a very small nugget effect, without the possibility to precise its value.

A display of the data shows an essentially linear NW–SE global trend (Figure 2). Not surprisingly, the raw variogram is clearly parabolic (Figure 3a). The directional variograms (not reproduced here) show, however, that no direction is entirely free of drift.



**FIGURE 2.** Display of microgravimetry data. The domain is a square of 384m  $\times$  384m. The Bouguer anomaly varies between  $-50$  and  $2450 \mu\text{gal}$ ; "C" represents the lowest values, and "3" represents the largest values.

Because the drift has a simple overall shape, a sensible approach is to work with the variogram of the residuals obtained after subtraction of a polynomial least-squares trend. This variogram is only slightly biased at small distances, and knowledge of the variogram at small distances is enough for a subsequent kriging in moving neighborhood. Local variograms of the residuals were computed in subdomains. They are quite isotropic and present no significant variations through the study domain. Therefore, we worked with global omnidirectional variograms. The least-squares trend and the variogram of the residuals have been computed with the data of the regular grid, to avoid giving more weight to specific areas. Figures 3b–d show the variograms of residuals  $\gamma_1$ ,  $\gamma_2$ , and  $\gamma_3$  associated with trends of degree 1, 2, and 3, respectively.



**FIGURE 3.** Microgravimetry in a quarry: (a) raw variogram; and variogram of residuals obtained after subtracting a global drift of degree  $k$  estimated by least squares: (b)  $k = 1$ ; (c)  $k = 2$ ; (d)  $k = 3$ . Notice the change in vertical scale between the raw variogram and the variograms of residuals.

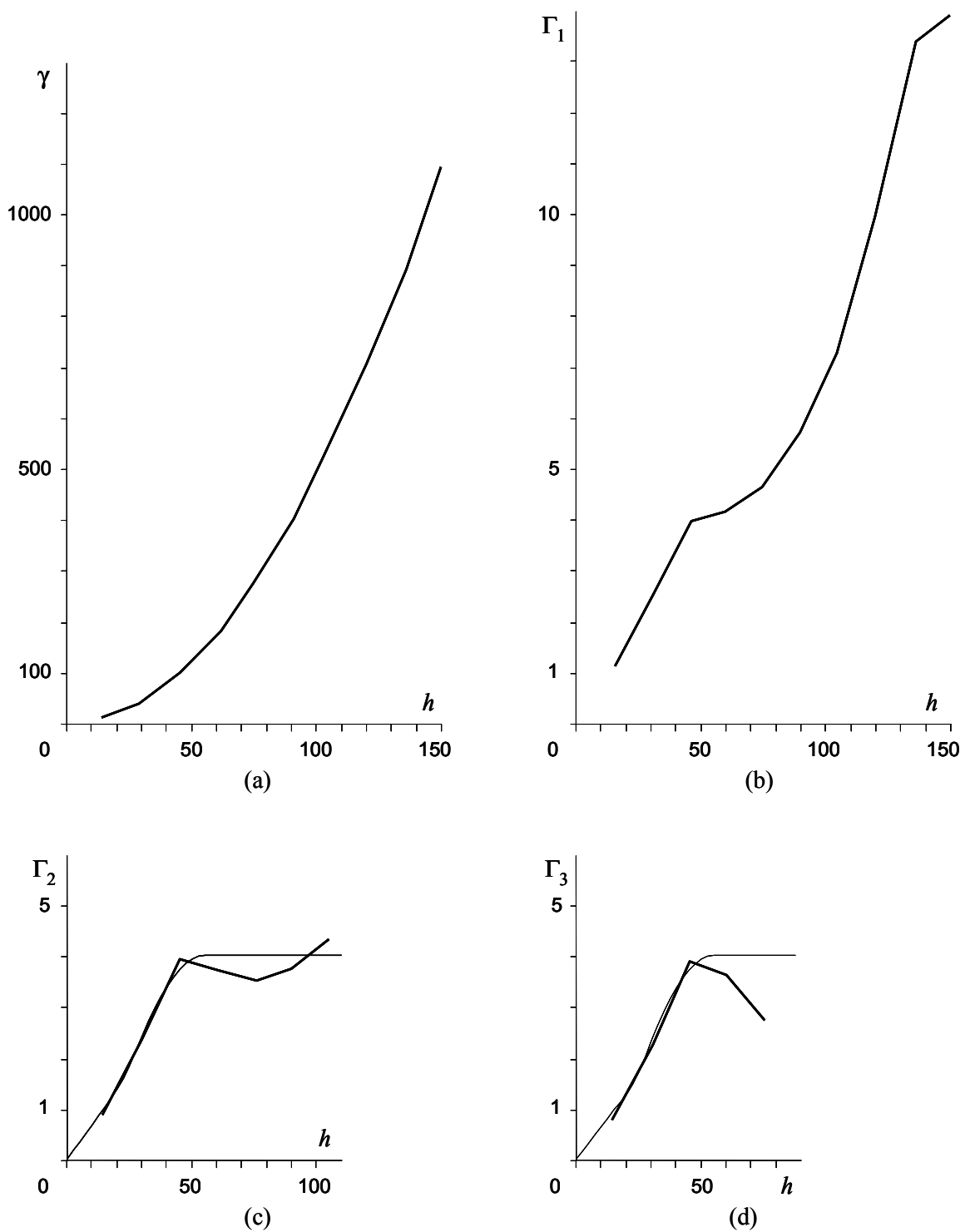
They show that in order to eliminate the effect of the drift, we must consider a global drift of degree 2, if not 3. The variogram of residuals then has a range of 60 m, or about one-sixth of the length of the domain. In this case the variogram of residuals is practically unbiased up to half the length of the domain (this is apparent when constructing simulations without drift, subtracting a least-squares trend, and comparing the raw variogram with the variogram of residuals). We obtain a good fit of  $\gamma_3$  by a spherical model with range  $a = 60$  m and sill  $C = 430 \mu\text{gal}^2$ , plus a measurement error nugget effect  $C_0 = 4 \mu\text{gal}^2$ . To cross-validate the fit, 146 sample points were estimated from their neighbors and gave a mean square standardized error (ratio of sample variance by theoretical estimation variance) of 1.06, which is excellent.

As the sampling is regular, the generalized variogram approach can also be applied. Figure 4a again displays the raw variogram (i.e., the sample GV of order 0) whereas Figures 4b–d display the sample generalized variograms  $\Gamma_1$ ,  $\Gamma_2$ , and  $\Gamma_3$  computed for  $k = 1, 2$ , and  $3$ , respectively, and averaged over the two main directions of the grid. Naturally, these variograms are computed up to the distance  $L / (k + 1)$ , where  $L$  is the length of the study domain.

They show quite clearly that the drift is still present in  $\Gamma_1$ , but filtered by  $\Gamma_2$  and  $\Gamma_3$ . One notices a range of about 50 meters. Using the curves of Figure 1,  $\Gamma_2$  can be fitted very well by the GV associated with the spherical model of range  $a = 55$  m and sill  $C = 400 \mu\text{gal}^2$ , plus the nugget effect  $C_0 = 4 \mu\text{gal}^2$ . This fit is also fine for  $\Gamma_3$ . The same cross-validation exercise as above gives a mean square standardized error of 1.04.

In this example, the generalized variogram gives practically the same results as the variogram of residuals (the slope at the origin changes by less than 1%). Note nevertheless that the GV fit was achieved with  $k = 2$  because generalized increments filter the drift locally, whereas  $k = 3$  was required with the variogram of residuals based on a global fit. An application to the topography of a fracture is provided by Chilès and Gentier (1993) and reproduced in Chilès and Delfiner (1999, pp. 279–280, or 2012, pp. 284–286). The drift has also a simple form, which allows a global fit, and the two approaches also lead to similar results. In more complex cases a simple global fit of the drift is not satisfactory. If the data are sampled along lines, then the generalized variogram has a role to play. At short distances it only involves close points and filters the local drift. In addition,  $\Gamma(h)$  can reflect the unbounded behavior of the underlying generalized covariance, while by construction the variogram of residuals is always bounded.





**FIGURE 4.** Microgravimetry in a quarry: generalized variogram of order  $k$ : (a)  $k = 0$  (i.e., variogram  $\gamma(h)$  identical to that of Figure 3a); (b)  $k = 1$ ; (c)  $k = 2$ ; (d)  $k = 3$ . Notice the change in vertical scale between the raw variogram and the generalized variograms.

## THEORY OF THE ESTIMATION OF THE GENERALIZED VARIOGRAM

We have defined a way for inferring the generalized covariance when regularly spaced data are available. This approach is based on the computation of the sample GV and on its fitting to a model. But are we sure that these operations can be performed under satisfactory conditions? Estimating and modeling the generalized variogram pose problems that pertain more to epistemology than to mathematical statistics. This is already the case with the ordinary variogram. In this context, these problems have attracted the attention of geostatisticians since the beginning (Matheron, 1965, Chapter XIII) and have fostered extensive studies (see Alfaro, 1979, and the methodological work of Matheron, 1978). This approach is presented in Chilès and Delfiner (1999, section 2.9). In this section we reproduce the results obtained by Alfaro and Matheron for the variogram and extend them in a straightforward manner to the generalized variogram (some early results can be found in Matheron, 1972).

In the sequel, the value  $k$  is fixed, and the subscript  $k$  is usually omitted.

### Regional GV and Sample GV

In practice, we consider a regionalized variable  $z(x)$  defined over a bounded domain  $D$ . By interpreting  $z(x)$  as a realization of a random function  $Z(x)$ , we have provided a theoretical definition (4) of the generalized variogram  $\Gamma(h)$ . Generally, however, the phenomenon under study is unique, and it is primarily the generalized variogram of the regionalized variable in  $D$  that is of interest. This GV is the regional GV defined by

$$\Gamma_R(h) = \frac{1}{M |D_h|} \int_{D_h} z_h(x)^2 dx \quad (9)$$

where:

- $z_h(x)$  is the increment of order  $k+1$ ,  $\Delta_h^{k+1} z(x)$ , defined by (3);
- $D_h$  represents the set of points  $x$  such that  $x + p h$ ,  $p = 0, 1, \dots, k$ , belong to  $D$  (i.e., such that  $z_h(x)$  is defined), and  $|D_h|$  is the measure (volume) of this set;
- $M$  stands for the norming factor  $M_k = \binom{2k+2}{k+1}$ .

The regional GV is a purely deterministic and empirical quantity. If we know  $z(x)$  at every point of  $D$ ,  $\Gamma_R$  is completely determined. It constitutes a summary of the structural characteristics of the regionalized variable and, in this sense, conveys a physical significance independently of the probabilistic interpretation that we can construct.

In practice,  $z(x)$  is only known at a finite number of sample points  $\{x_i : i = 1, 2, \dots, N\}$ . As the regional GV cannot be determined directly, we calculate the sample GV defined by

$$\hat{\Gamma}(h) = \frac{1}{M N_h} \sum_{i \in I_h} z_h(x_i)^2$$

where

- $I_h$  is the subset of all points  $x_i$  such that  $x_i + p h$ ,  $p = 0, 1, \dots, k$ , are data points (i.e., such that  $z_h(x_i)$  can be computed);
- $N_h$  is the number of elements of  $I_h$ .

Note that for  $k > 0$ ,  $\hat{\Gamma}(h)$  can only be computed in the case of regularly spaced data (on a grid or on lines), for  $h$  multiple of the data spacing.

### Estimation Variance of the Sample GV

An immediate question arises from the previous definitions: Is the sample GV a good approximation of the regional GV? An experimental answer to this question is only possible in the rare cases of an exhaustive survey. One such case—for an ordinary variogram—is Narboni's (1979) exhaustive survey of the Ngolo tropical forest (see Chilès and Delfiner, 1999, pp. 138–139, or 2012, pp. 139–140).

Exhaustive sampling situations are exceptional, and we must consider the general case where the regional GV  $\Gamma_R(h)$  cannot be determined experimentally. If we fix  $h$  and let

$$q_h(x) = \frac{1}{M} z_h(x)^2 = \frac{1}{M_k} \left[ \Delta_h^{k+1} z(x) \right]^2$$

we see that the expression (9) of  $\Gamma_R(h)$  is simply the average value of  $q_h(x)$  over  $D_h$ , and that  $\hat{\Gamma}(h)$  is the average value of the  $N_h$  data  $q_h(x_i)$ . It is reasonable to expect that if sufficient data are available and fairly well distributed,  $\hat{\Gamma}(h)$  is close to  $\Gamma_R(h)$ . If, for example, the data are on a regular grid, and if  $h$  is a multiple of the grid spacing,  $\hat{\Gamma}(h)$  is simply the discrete approximation of the integral defining  $\Gamma_R(h)$ .

To go further, we have to specify the behavior of the regionalized variables  $z(x)$  and  $q_h(x)$ . In our models we interpret  $z(x)$  as a realization of a random function  $Z(x)$ , and then  $q_h(x)$  is a realization of the random function

$$Q_h(x) = \frac{1}{M} Z_h(x)^2 \quad (10)$$

We assume here that  $Z(x)$  is an IRF- $k$  with GC  $K(h)$ , so that  $Z_h(x)$  is an (order-2) SRF. We also assume that the random function  $Q_h(x)$  has second-order moments and is stationary. Let  $G_h(x' - x)$  denote the covariance of  $Q_h(x)$  and  $Q_h(x')$ . To avoid weighting down the notation,  $\Gamma_R$  and  $\hat{\Gamma}$  will now designate the random versions of the regional GV and the sample GV, or explicitly:

$$\Gamma_R(h) = \frac{1}{|D_h|} \int_{D_h} Q_h(x) dx \quad (11)$$

$$\hat{\Gamma}(h) = \frac{1}{N_h} \sum_{i \in I_h} Q_h(x_i) \quad (12)$$

Naturally,

$$E[\Gamma_R(h)] = E[\hat{\Gamma}(h)] = \Gamma(h)$$

since  $Q_h(x)$  has for expectation  $\Gamma(h)$ . We can thus characterize the error incurred by taking the sample GV for the regional GV by the variance of  $\hat{\Gamma}(h) - \Gamma_R(h)$ . Considering the respective definitions of each term (average of  $N_h$  values  $Q_h(x_i)$  for one, average of  $Q_h(x)$  over  $D_h$  for the other) brings us back to a standard calculation of estimation variance to be carried out with the covariance  $G_h(x' - x)$  of the SRF  $Q_h(x)$ :

$$\begin{aligned} \text{Var}[\hat{\Gamma}(h) - \Gamma_R(h)] &= \frac{1}{|D_h|^2} \int_{D_h} \int_{D_h} G_h(x' - x) dx dx' - \frac{2}{N_h |D_h|} \sum_{i \in I_h} \int_{D_h} G_h(x - x_i) dx \\ &\quad + \frac{1}{N_h^2} \sum_{i \in I_h} \sum_{j \in I_h} G_h(x_j - x_i) \end{aligned} \quad (13)$$

$G_h(x' - x)$ , however, is a fourth-order moment of ALC- $k$ 's of the IRF- $k$   $Z(x)$ . Determining the precision of the calculation of the second-order moment thus requires prior knowledge of the fourth-order moment. But the latter can generally be evaluated with mediocre precision, related to the eighth-order moment, and so on. This way the problem can be displaced endlessly. We can nevertheless determine orders of magnitude by considering classic cases of spatial distribution. The Gaussian case will be examined first, and then indications will be given for SRFs with skewed marginal distributions.

### Estimation Variance in the Gaussian Case

As demonstrated in Appendix A, in the case of a Gaussian IRF- $k$ , the covariance of  $Q_h$  is directly derived from the covariance of  $Z_h$ :

$$G_h(x' - x) = \frac{2}{M^2} C_h(x' - x)^2 \quad (14)$$

where  $C_h(l)$  is the covariance defined in (6) and expressed by (7) in terms of the GC  $K(h)$ .

In case of regularly located data, the estimation variance is essentially linked with the irregular—that is, uneven—terms of lower degree of the covariance in the vicinity of the origin. As demonstrated in Appendix B, the estimation variance can be computed, to a first approximation, as if the variogram of  $Q_h$  behaved as  $4 \Gamma(h) [K(x' - x) - K(0)]$ . As a consequence, for 1D data with spacing  $d$ , the relative estimation variance is

$$S_E^2(h) = \frac{\text{Var}[\hat{\Gamma}(h) - \Gamma_R(h)]}{\Gamma(h)^2} \simeq \frac{4}{\Gamma(h)} \frac{\sigma_d^2}{N_h}$$

where  $\sigma_d^2$  is the estimation variance of the elementary mesh by its central value for a variable whose covariance has the same irregular terms as  $K(\cdot)$  near the origin, and where  $N_h$  is the number of available increments of order  $k + 1$ . Thus, provided that  $N_h$  is large enough, we are

sure of being able to evaluate  $\Gamma_R(h)$  with good precision:  $\hat{\Gamma}$  is a consistent estimator of  $\Gamma_R$ . Appendix B gives further results concerning a power-law behavior.

Alfaro (1979) has computed  $S_E^2(h)$  in the case of a variogram ( $k = 0$ ) for data sets of 21 points in 1D and  $5 \times 5$  points in 2D. We have carried out similar computations with an improved precision, an extension to a GV of order 1, 2, or 3, and a larger number of data (program MARKO; source code of 1989 in Appendix D). Figure 5 presents the relative estimation standard deviation  $S_E(h)$  for  $k = 0$  and a spherical or power-law variogram. The top of the figure is the 1D case: A segment of length  $L$  is sampled regularly by 121 data points. The bottom of the figure is the 2D case: A square  $L \times L$  is sampled by a grid of  $13 \times 13$  data points. Figures 6 and 7 present similar results for  $k = 1$  and 2, respectively. The horizontal scale is adapted to the largest possible lag  $L / (k + 1)$  for  $\Gamma_R$  and  $\hat{\Gamma}$ . These figures show that:

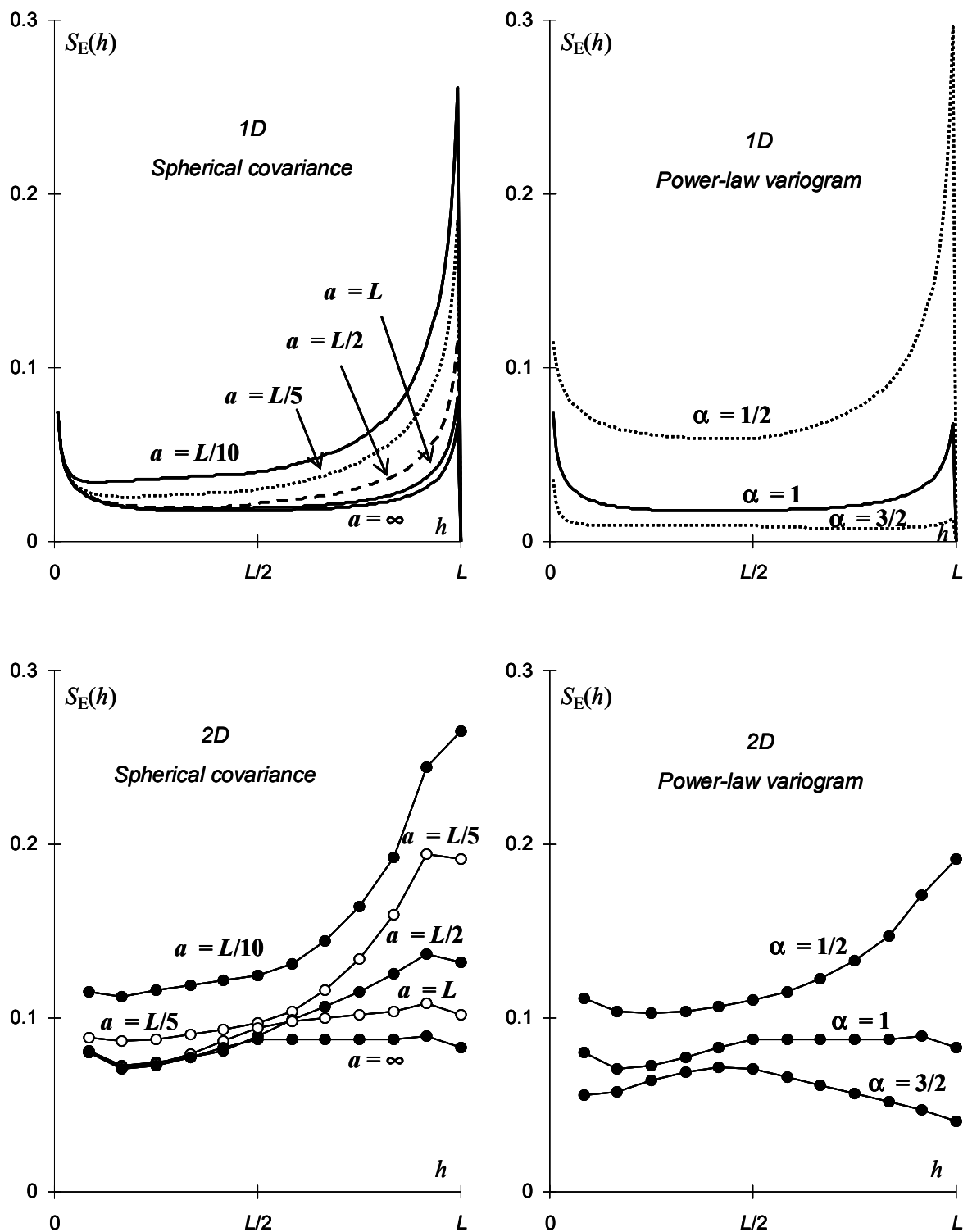
- The precision improves with the regularity of the GC (large range or high power  $\alpha$ ).
- In  $\mathbb{R}^2$ , the precision is practically of the same order of magnitude for all values of  $h$  (except when  $h$  reaches the domain size), whereas in  $\mathbb{R}^1$  it is better for medium distances than for small distances.
- The precision decreases only slightly when the degree  $k$  increases; let it be recalled that  $\Gamma(h)$  gives information about  $K(h), K(2h), \dots, K((k + 1)h)$ .
- Quantitatively,  $S_E(h)$  is usually of the order of 10%, which can be considered satisfactory due to the limited number of data considered here.

### Estimation Variance in the General Case

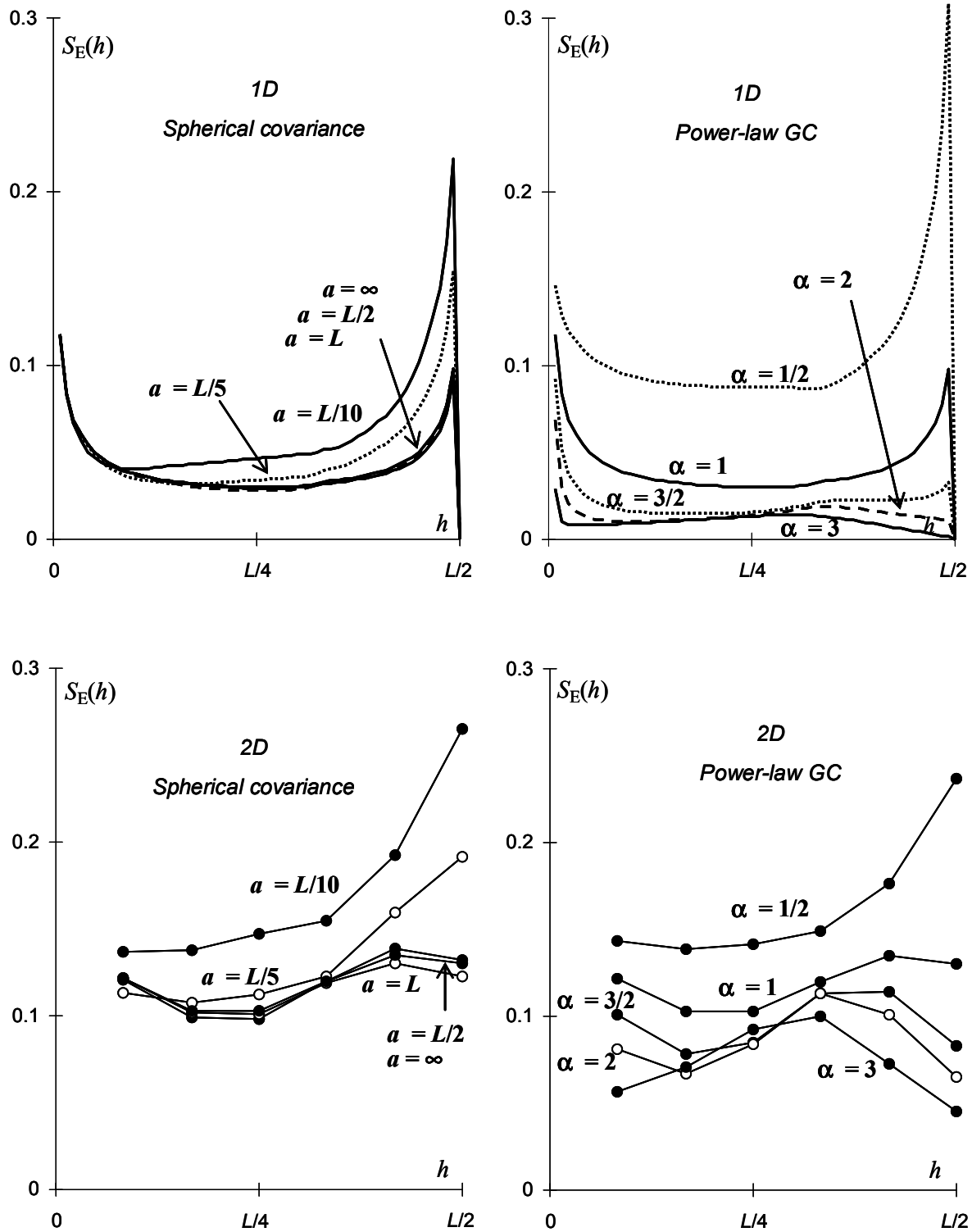
To give a glimpse of the precision that one can expect with non-Gaussian random functions, let us consider the case  $k = 0$  with three different SRFs already considered by Alfaro (1979), with an exponential covariance  $K(h) = C e^{-|h|/a}$ . These SRFs are derived from independent standard Gaussian SRFs  $U(x)$  and  $V(x)$  with the same correlogram  $\rho(h)$ :

- i)  $Z_1(x) = U(x)V(x)$ : Its marginal distribution has the probability density function  $f(z) = \frac{1}{\pi} K_0(|z|)$ , where  $K_0$  is the order-0 Bessel function of the second kind. Its covariance is  $C(h) = \rho(h)^2$ .
- ii)  $Z_2(x) = U(x)^2$ : Its marginal distribution is gamma with parameters 1/2 and 1/2 (chi-square distribution on one degree of freedom). Its covariance is  $C(h) = 2\rho(h)^2$  and its coefficient of variation is  $\sqrt{2} \approx 1.414$ .
- iii)  $Z_3(x) = e^{U(x)}$ : It is a lognormal SRF with covariance  $C(h) = e(e^{\rho(h)} - 1)$ , thus with a fairly high coefficient of variation  $\sqrt{e-1} \approx 1.311$ .

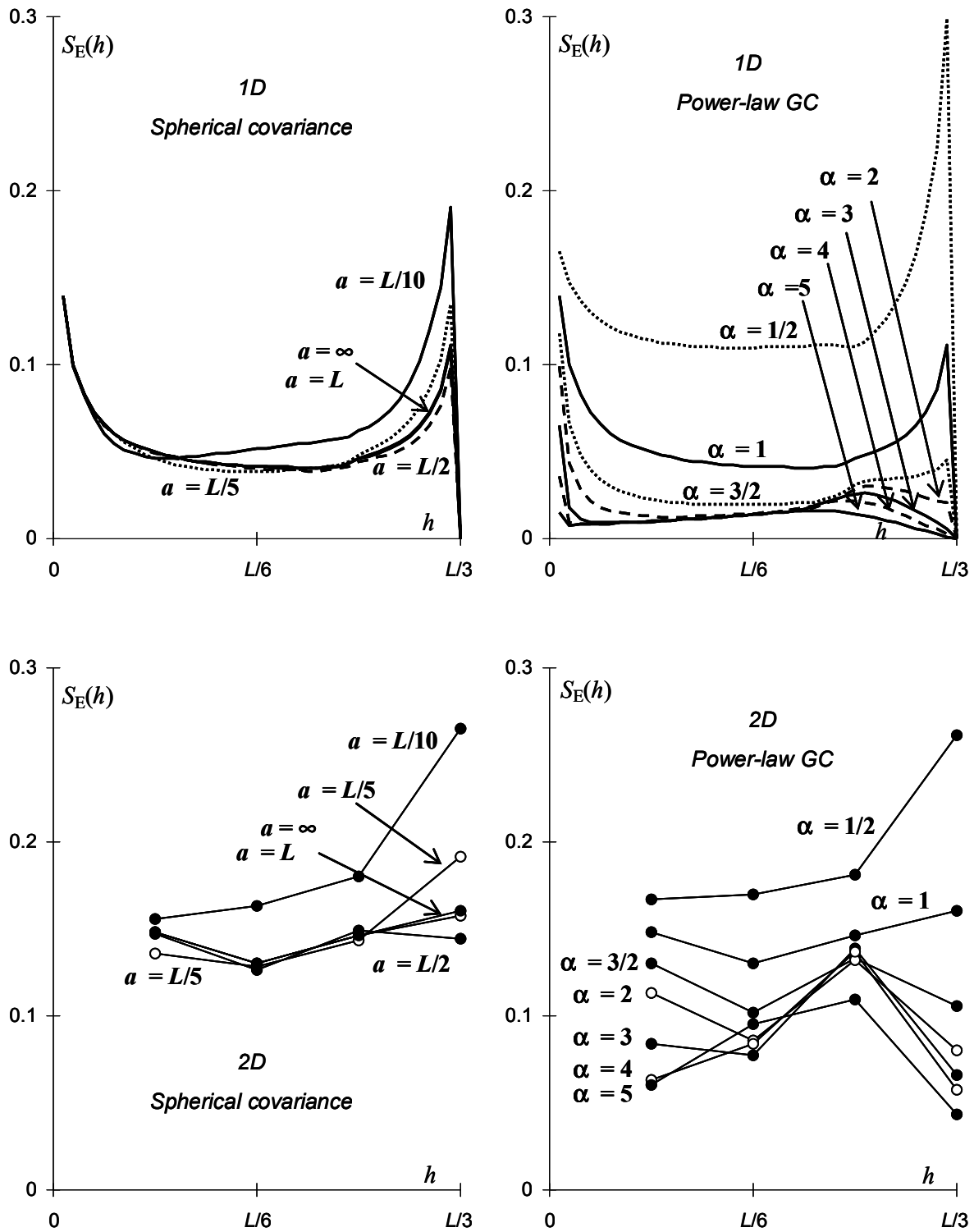
The three random functions have been selected because it is not too difficult to calculate the covariance  $G_h(x' - x)$  from the results relative to Gaussian random variables—at least when  $k = 0$  (Alfaro, 1979). The expression of  $G_h(x' - x)$  for these three random functions is given in Appendix A.



**FIGURE 5.** Estimation of the regional variogram: relative standard deviation  $S_E(h)$  in the Gaussian case for a spherical covariance with range  $a$  (on the left) and for a variogram of type  $|h|^\alpha$  (on the right). Top: 121 points sample a segment of length  $L$ . Bottom:  $13 \times 13$  points sample a square  $L \times L$ .

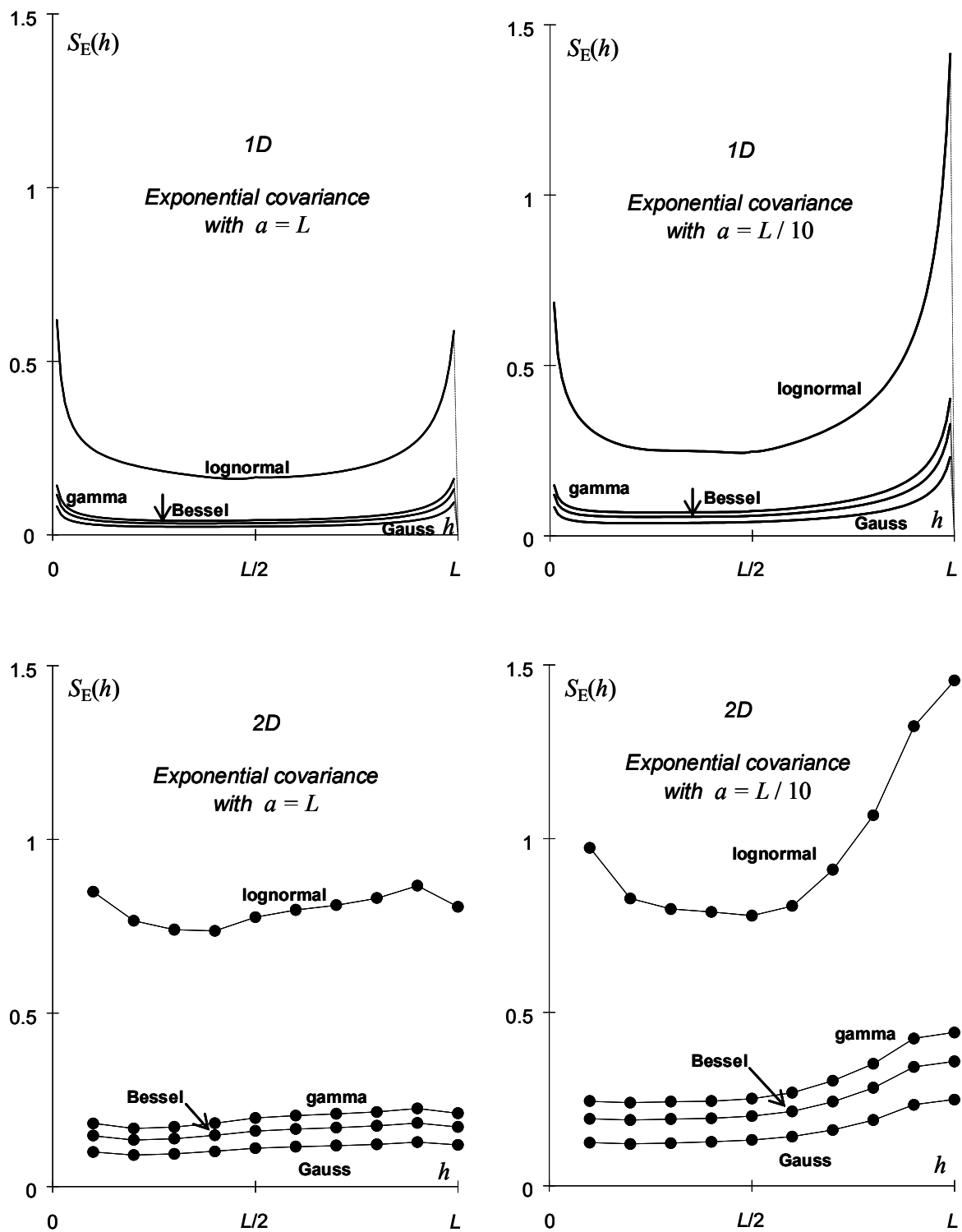


**FIGURE 6.** Estimation of the regional GV of order 1: relative standard deviation  $S_E(h)$  in the Gaussian case for a spherical covariance with range  $a$  (on the left) and for a power-law or power-logarithmic GC with shape parameter  $\alpha$  (on the right). Top: 121 points sample a segment of length  $L$ . Bottom:  $13 \times 13$  points sample a square  $L \times L$ .



**FIGURE 7.** Estimation of the regional GV of order 2: relative standard deviation  $S_E(h)$  in the Gaussian case for a spherical covariance with range  $a$  (on the left) and for a power-law or power-logarithmic GC with shape parameter  $\alpha$  (on the right). Top: 121 points sample a segment of length  $L$ . Bottom:  $13 \times 13$  points sample a square  $L \times L$ .





**FIGURE 8.** Estimation of the regional variogram: relative standard deviation  $S_E(h)$  for different spatial distributions, for an exponential variogram with scale parameter  $L$  (on the left) and  $L/10$  (on the right). Top: 101 points sample a segment of length  $L$ . Bottom:  $11 \times 11$  points sample a square  $L \times L$ .

An exponential covariance has been considered, because it is very easy to obtain it in the first two cases ( $\rho(h)$  must also be exponential, with twice the scale parameter of  $C(h)$ ). As for the lognormal SRF, we have used a correlogram  $\rho(h)$  giving a covariance  $C(h)$  as close as possible to the exponential model (an exponential model with variance 0.5 and scale parameter  $1.6a$ , plus a spherical model with variance 0.5 and range  $2.7a$ , where  $a$  is the desired scale parameter for  $C(h)$ ).

The calculations have been carried out with the program MARCO (source code of 1989 in Appendix E). Figure 8 presents the relative estimation standard deviation  $S_E(h)$  for two different values of the scale parameter and for sampling schemes similar to those considered in Figure 5, except that we now have 101 data points in 1D or  $11 \times 11$  data points in 2D. As in the similar study carried out by Alfaro (1979), it shows that:

- The sample variogram is less precise than in the Gaussian case.
- It is acceptable for distributions such as those of  $Z_1$  and  $Z_2$  which are not too long tailed.
- The sample variogram of a variable with a long-tailed distribution, like  $Z_3$ , bears only a distant relationship to the regional variogram. Besides, this last result is linked with a well-known phenomenon: a proportional effect.

### **Conclusions on the Estimation of the GV**

The precision of the estimation of a GV is similar to that of an ordinary variogram. It is satisfactory in the Gaussian case. Like for the calculation of an ordinary variogram, inhomogeneities in the studied domain or in the data must be taken into account. In case of variables whose increments  $Z_h(x)$  have strongly non-Gaussian distributions (especially long tails), the precision of the sample GV may be very poor. Robust techniques can transform the data into a more regular variable (logarithmic transformation, for example). Robust techniques developed for the ordinary variogram calculation can be directly transposed to the GV (see, e.g., Cressie, 1991; Chilès and Delfiner, 1999, section 2.2.5). But let it be borne in mind that the applications usually need the GV of  $Z(x)$  and not of some smoother variable.

## **THEORY OF THE FLUCTUATION OF THE GENERALIZED VARIOGRAM**

### **Fluctuation Variance of the Regional GV**

Even if we knew the value of the regionalized variable  $z(x)$  at every point of the studied domain  $D$  and were capable of calculating the regional GV  $\Gamma_R(h)$  for any vector  $h$ , this would exhibit so many variations of detail that we would have to simplify it to be able to express it in a usable form. That amounts to considering that two very similar regional GVs have the same parent GC  $K(h)$  and GV  $\Gamma(h)$ . This simplification represents exactly a passage to the mathematical expectation: If one considers the studied regionalized variable as the realization of an IRF- $k$ , namely as one realization among a set of similar realizations, the regional GV of the regionalized variable is one among a family of regional GVs whose mean, or in probabilistic terms mathematical expectation, is a theoretical GV  $\Gamma(h)$ .

The passage to the IRF- $k$  model enables us to define criteria for the precision required during modeling. In the framework of this model, the deviation  $\Gamma_R(h) - \Gamma(h)$  is a random variable. Its expectation is zero, and we can quantify the possible deviations by the fluctuation variance  $\text{Var}[\Gamma_R(h) - \Gamma(h)]$ . Let us therefore consider a given value of  $h$  and use the notations of the previous section. In view of definition (11) of  $\Gamma_R(h)$ , the variance of the fluctuation of  $\Gamma_R(h)$  is simply the variance of the fluctuation of the mean of  $Q_h(x)$  in  $D_h$ . It can therefore be expressed in terms of the covariance  $G_h(x' - x)$  of the SRF  $Q_h(x)$ :

$$\text{Var}[\Gamma_R(h) - \Gamma(h)] = \frac{1}{|D_h|^2} \int_{D_h} \int_{D_h} G_h(x' - x) dx dx' \quad (15)$$

Calculating this variance again involves the fourth-order moment of the IRF- $k$   $Z(x)$ . Given the same remarks as in the preceding section, let us first examine the Gaussian case.

### Fluctuation Variance in the Gaussian Case

In view of the expression (14) for  $G_h(x' - x)$  in the Gaussian case, (15) is expressed as a function of  $C_h(\cdot)$ :

$$\text{Var}[\Gamma_R(h) - \Gamma(h)] = \frac{2}{|D_h|^2} \int_{D_h} \int_{D_h} C_h(x' - x)^2 dx dx'$$

The explicit calculation is complex, so for simplification we will first consider the case where  $K(x' - x)$  near the origin is equivalent to  $(-1)^{1+\lfloor \alpha/2 \rfloor} b |x' - x|^\alpha$  (again the even terms up to degree  $2k$  have no influence on the GV and are not considered here). Matheron (1978, p. 113) has stated that for small  $h$ , the relative fluctuation variance is, to a first approximation, of the form

$$S_F^2(h) = \frac{\text{Var}[\Gamma_R(h) - \Gamma(h)]}{\Gamma(h)^2} \simeq A |h|^{4k+4-2\alpha} + B |h|^n$$

where  $n$  is the dimension of the space (1, 2, or 3) (in fact Matheron considers the case  $k = 0$ ; he gives the proof in  $\mathbb{R}^1$  in Matheron, 1970, section 2.10.3; the proof in  $\mathbb{R}^n$  for  $k \geq 0$  is given in Appendix C). This relative variance tends to zero with  $|h|$  if and only if  $\alpha < 2k + 2$ .

### Micro-Ergodicity

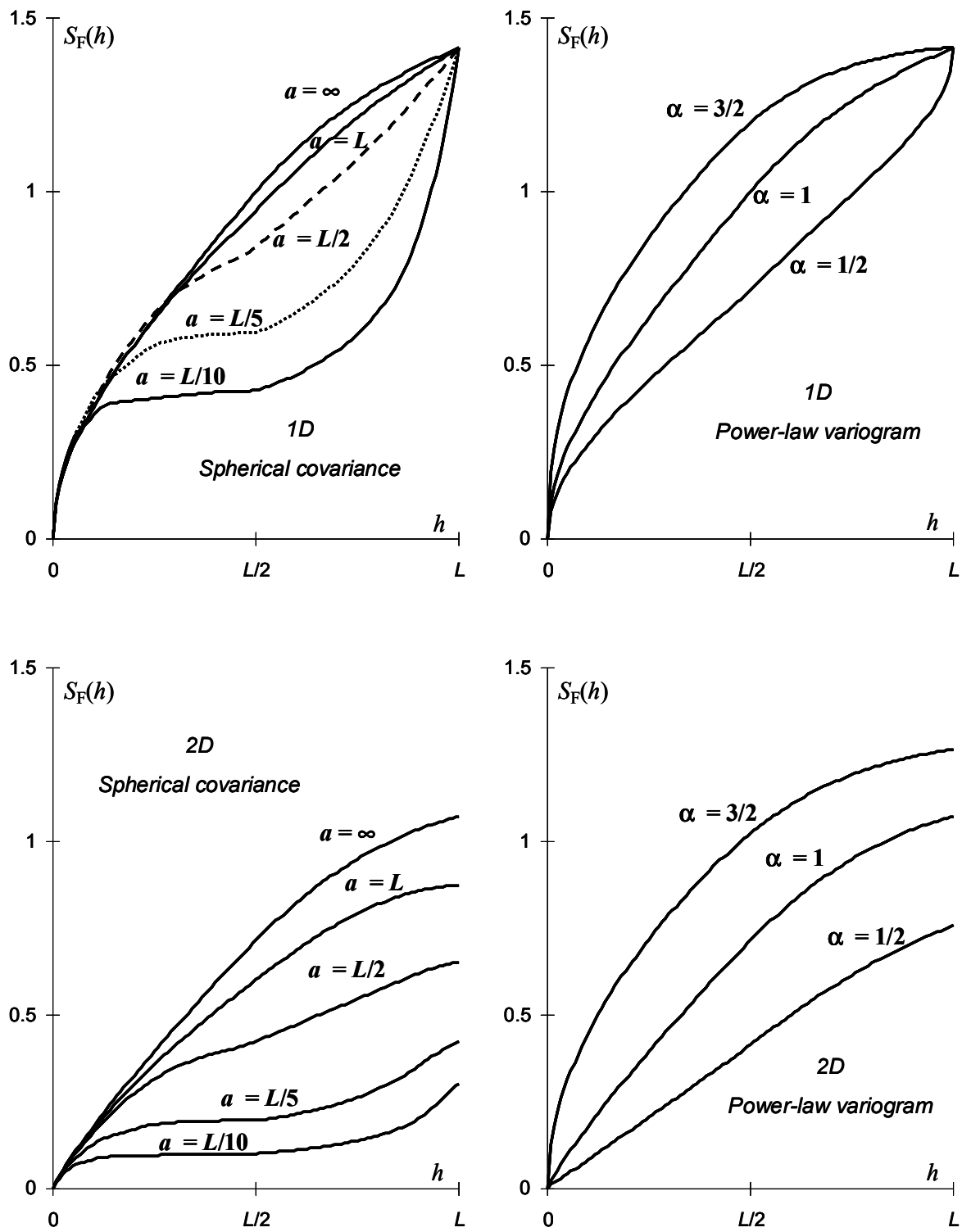
In the above situation, the convergence of  $\Gamma_R(h) / |h|^\alpha$  to a constant  $b' = B_\alpha b$  when  $h \rightarrow 0$  is ensured, provided that the IRF- $k$   $Z(x)$  is not differentiable  $k + 1$  times ( $B_\alpha$  is given by (8)). The parameter  $b$  then has an objective meaning: If we increase the number of sample points by refining the sampling grid, we can estimate it with precision. This is the concept of micro-ergodicity, introduced by Matheron (1978, pp. 109–114); Cressie, 1991, calls this “infill asymptotics”). It differs from conventional ergodicity, where one extends the data domain to infinity, which is of little interest to us because we always work in a bounded domain  $D$ .

The micro-ergodicity of the GV in the neighborhood of the origin is therefore established, provided that  $K(h)$  is not too regular (we find ourselves in an inverse situation to that of the estimation of the regional GV). This is easily explained: If the IRF- $k$  is differentiable  $k + 1$  times, it admits a local expansion with a polynomial of degree higher than  $k$ —that is, the residuals are more regular than the drift. In this case, the model is not adapted, and it is advisable to use either a higher degree  $k$  or a deterministic model (at least at the scale of a small domain). A well-known example is the Gaussian covariance  $K(h) = \exp(-|h|^2/a^2)$ , which is indefinitely differentiable and can be developed as an infinite sum of even terms.

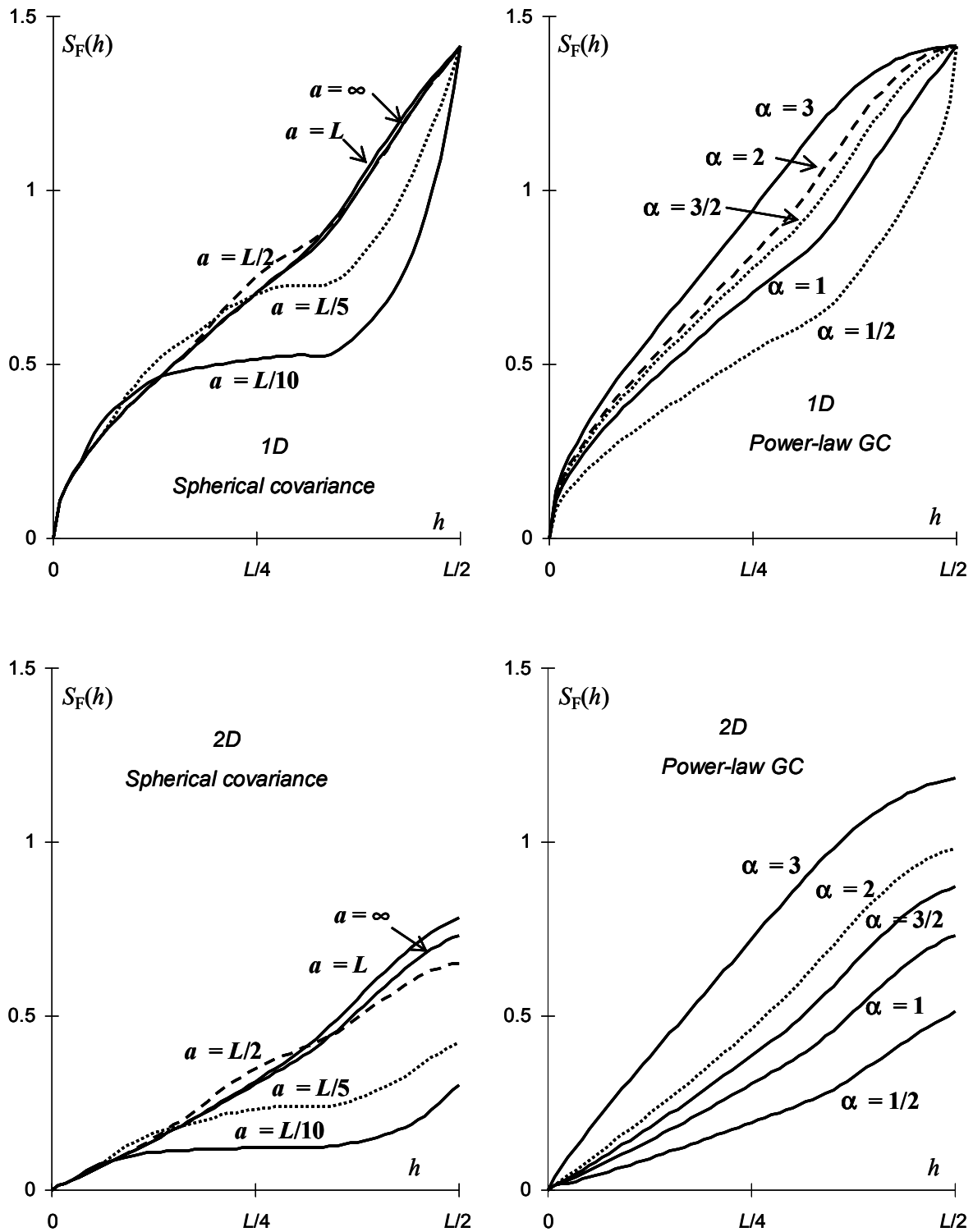
In geostatistical applications, the condition  $\alpha < 2k + 2$  concerning the behavior of  $K(h)$  near the origin is usually met (note that it coincides with the condition for  $(-1)^{1+\lfloor \alpha/2 \rfloor} |h|^\alpha$  to be a GC from  $h = 0$  to infinity). So the determination of  $\Gamma(h)$  in the neighborhood of the origin is possible. On the other hand, the fluctuation variance increases very rapidly with  $h$  (except if  $K(h)$  has a very small range with respect to the domain  $D$ ).

Figures 9, 10, and 11 show the relative fluctuation standard deviation curves  $S_F(h)$  for  $k = 0, 1,$  and  $2$ , respectively, for the same GC models as in Figures 5 to 7 for the relative estimation standard deviation curves  $S_E(h)$ . The computations were carried out with program MARKO (Appendix D) by discretizing the domain  $D$  by 1201 points in 1D and by  $121 \times 121$  points in 2D. It can be observed that:

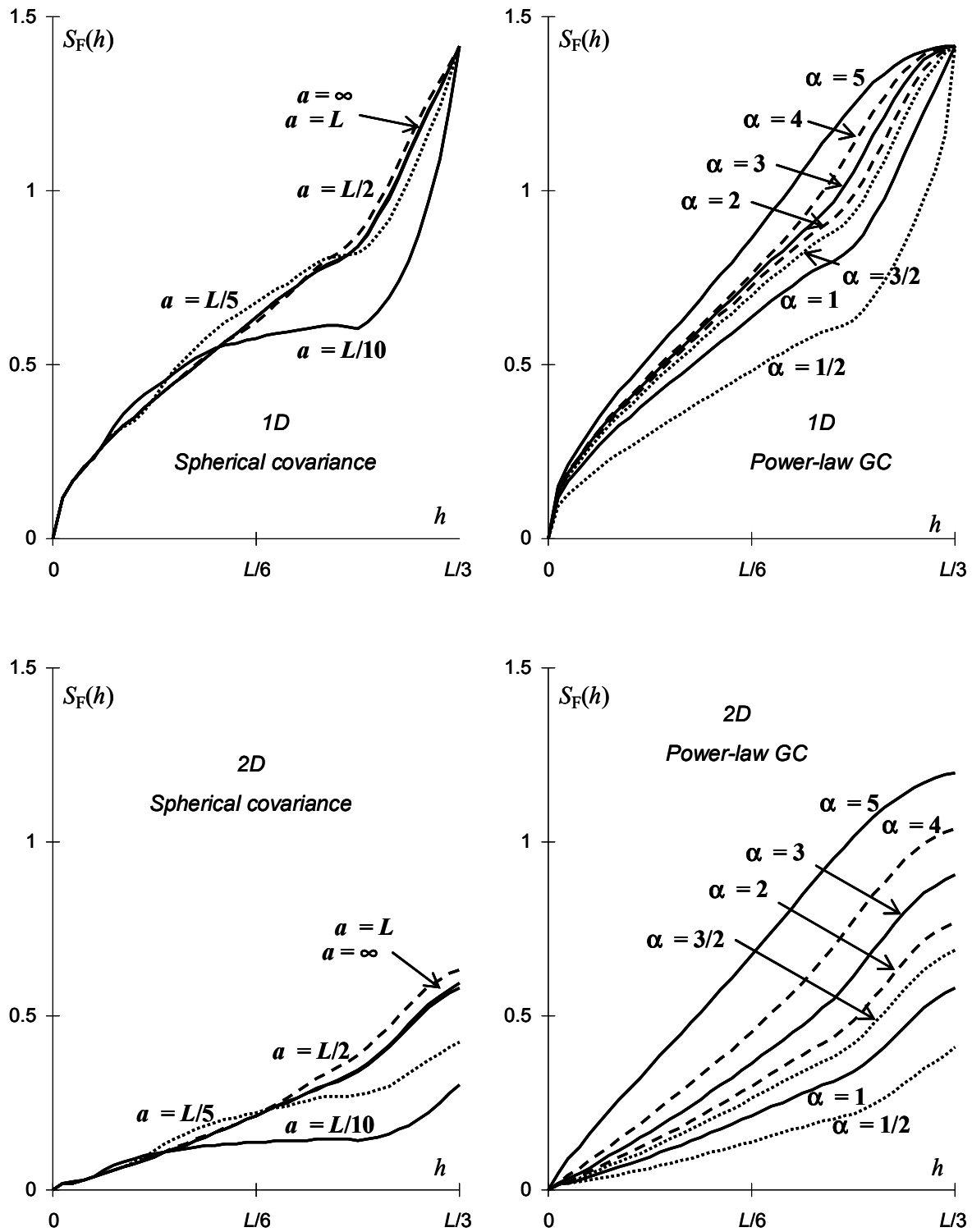
- In the 1D case, all the curves rise from 0 for  $h = 0$  to 2 for  $h = L / (k + 1)$ , as at this distance only one increment is available for calculating  $\Gamma(h)$ .
- The more regular the GC (large range or high  $\alpha$ ), the larger the fluctuations; on the contrary, in the limit case of a pure nugget effect, the fluctuation variance is zero, except for  $h = L / (k + 1)$ . Note that this observation is the opposite to that made about the estimation of the GV.
- The possible fluctuations in  $\mathbb{R}^2$  are not as strong as in  $\mathbb{R}^1$ . This is a nice property because most geostatistical applications are in 2D or even in 3D.
- The fluctuations increase with the degree  $k$ , mainly because the maximum distance for computing  $\Gamma_R(h)$  is the size of the domain divided by  $k + 1$ .
- Even in  $\mathbb{R}^2$ , apart from the case of a small range, the theoretical GV and the regional GV may have only a distant relationship if  $|h|$  is greater than half the maximum distance of possible computation of the regional GV (if not sometimes less). This is not serious insofar as geostatistical estimations depend much more on the behavior of the GC at small distances than at large distances. From a practical point of view, we can accept that the GV generally has no objective meaning at large distances and that it is pointless to try to refine the associated fit.



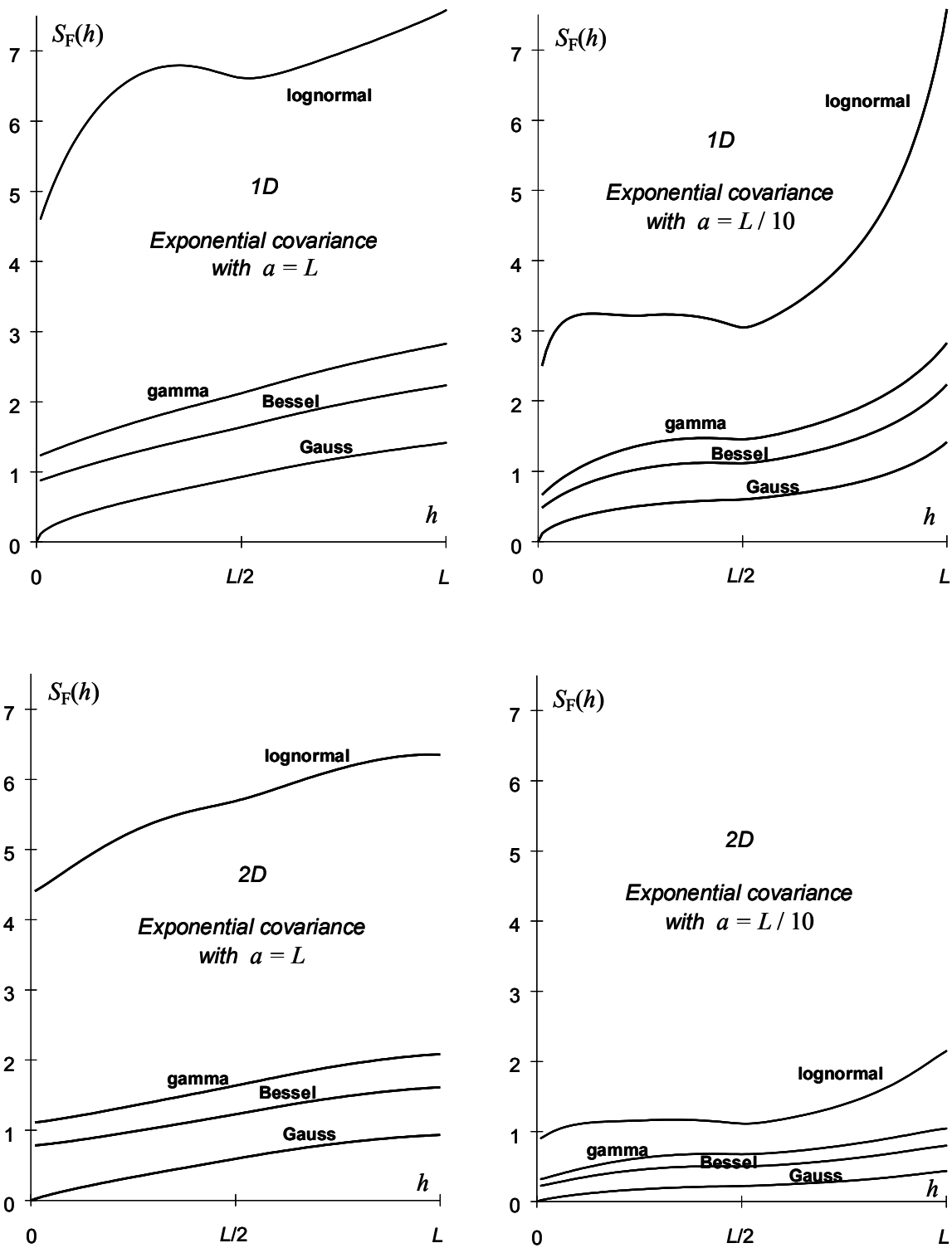
**FIGURE 9.** Fluctuation of the regional variogram: relative standard deviation  $S_F(h)$  in the Gaussian case for a spherical covariance with range  $a$  (on the left) and for a variogram of type  $|h|^\alpha$  (on the right). Top: the domain is a segment of length  $L$ . Bottom: the domain is a square  $L \times L$ .



**FIGURE 10.** Fluctuation of the regional GV of order 1: relative standard deviation  $S_F(h)$  in the Gaussian case for a spherical covariance with range  $a$  (on the left) and for a power-law or power-logarithmic GC with shape parameter  $\alpha$  (on the right). Top: the domain is a segment of length  $L$ . Bottom: the domain is a square  $L \times L$ .



**FIGURE 11.** Fluctuation of the regional GV of order 2: relative standard deviation  $S_F(h)$  in the Gaussian case for a spherical covariance with range  $a$  (on the left) and for a power-law or power-logarithmic GC with shape parameter  $\alpha$  (on the right). Top: the domain is a segment of length  $L$ . Bottom: the domain is a square  $L \times L$ .



**FIGURE 12.** Fluctuation of the regional variogram: relative standard deviation  $S_F(h)$  for different spatial distributions, for an exponential variogram with scale parameter  $L$  (on the left) and  $L/10$  (on the right). Top: the domain is a segment of length  $L$ . Bottom: the domain is a square  $L \times L$ .



## Fluctuation Variance in the General case

The conclusions are less encouraging for random functions that are clearly non-Gaussian, as has been shown by Alfaro (1979). Taylor expansions show that the behavior of  $S_F^2(h)$  at the origin is

$$- \text{ gamma SRF } Z_1(x): \quad S_F^2(h) = 2\frac{a}{L} - \frac{a^2}{L^2}(1 - e^{-2L/a}) \quad h \ll L$$

$$- \text{ Bessel SRF } Z_2(x): \quad S_F^2(h) = \frac{a}{L} - \frac{a^2}{2L^2}(1 - e^{-2L/a}) \quad h \ll L$$

$$- \text{ lognormal SRF } Z_3(x): \quad S_F^2(h) = \frac{e^4 a}{2L} \approx 27.30 \frac{a}{L} \quad h \ll L$$

These values are not equal to zero, so that these SRFs are not micro-ergodic. To obtain a small fluctuation variance, let say 0.01 (that is,  $S_F(h) < 0.1$ ), we need  $L = 200 a$  for the gamma SRF,  $L = 100 a$  for the Bessel SRF, and  $L = 2730 a$  for the lognormal SRF, that is, totally unreasonable values (there is little chance that an application conforms to a stationary model over such a domain). For  $h = L$ ,  $S_F^2(L)$  is equal to 8 for the gamma SRF, 5 for the Bessel SRF, in comparison to 2 for a Gaussian SRF. For the lognormal SRF,  $S_F^2(L)$  depends on  $\rho(L)$ ; it is equal to  $(e+1)(e^3 + e^2 + 2e - 2)/2 \simeq 57.47$  if  $\rho(L) = 0$ .

This is confirmed by Figure 12, which shows the results obtained for the same IRF-0's as in Figure 8. The computations were carried out with program MARCO (Appendix E) by discretizing the domain  $D$  by 1001 points in 1D and by  $101 \times 101$  points in 2D. Two conclusions can be drawn:

- The fluctuation variance can be much larger than in the Gaussian case.
- The relative variance no longer necessarily tends to zero when the lag  $h$  tends to zero: In other words, micro-ergodicity is no longer ensured, and the regional GV does not even reproduce the behavior near the origin of the theoretical GV.

## Conclusions on the Fluctuations of the Regional GV

The possible fluctuations of the regional GV are similar to those of an ordinary variogram. They are sufficiently small, at short distances, to ensure micro-ergodicity when the variable is more or less Gaussian. On the contrary, micro-ergodicity is not achieved for strongly non-Gaussian variables.

In practice, a lack of micro-ergodicity is frequently reflected in a proportional effect. If we treat it as such, which amounts to working on a variable conditioned on its local mean, we end up with a more satisfactory model. It is generally better to use methods based on prior transformation of the data into Gaussian variables (lognormal kriging, disjunctive kriging). Micro-ergodicity is also no longer ensured for an indicator, or more generally for a mosaic RF (even if the marginal distribution is Gaussian): If the study domain  $D$  is not large, a realization can very well be constant and thus give a regional variogram that is identically zero.

## CONCLUSION

The generalized variogram is an operational tool for modeling nonstationary phenomena. It has the advantages of the ordinary variogram: The sample GV can be calculated, displayed, interpreted in terms of behavior at the origin and at long distances, fitted graphically according to a generalized covariance model. Its link with the generalized covariance is very simple. In particular the polynomial/logarithmic GC model with nugget effect corresponds to a polynomial generalized variogram with positive coefficients. The limitation to the use of the generalized variogram is the required data configuration: data on grids or along profiles. This condition is nevertheless fulfilled in many situations. Applications are of two types:

- i) identification of the generalized covariance: Apart the case study presented above, see Chilès and Gable (1984) for geothermal data, and Chilès and Gentier (1993) for the topography of a single fracture.
- ii) check of geostatistical simulations: Examples are provided by Orfeuil (1972) and by Pardo-Igúzquiza and Dowd (2003).

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## APPENDIX A

### EXPRESSION OF $G_h(x' - x)$

As in the section on the inference of the GV, a given degree  $k$  is considered and the notational dependence on  $k$  is skipped.

By definition,  $G_h(x' - x)$  is the covariance of the SRF  $Q_h(x) = \frac{1}{M} Z_h(x)^2$ , where  $Z_h(x) = \Delta_h^{k+1} Z(x)$  is the increment of order  $k + 1$  defined by (3), and  $M$  is the norming factor  $M_k = \binom{2k+2}{k+1}$ . As  $G_h(x' - x)$  is a fourth-order moment of the IRF- $k$   $Z(x)$ , it depends not only on the GC  $K(h)$  but also on the spatial distribution of  $Z(x)$ .

#### Multi-Gaussian Case

The calculation of  $G_h(x' - x)$  in the multi-Gaussian case is based on the following property:

If  $U_1, U_2, U_3, U_4$  are  $\mathcal{N}(0, 1)$  random variables, with correlation coefficients  $\rho_{ij}$ , and if the random vector  $(U_1, U_2, U_3, U_4)'$  is Gaussian, then

$$E[U_1 U_2 U_3 U_4] = \rho_{12} \rho_{34} + \rho_{13} \rho_{24} + \rho_{14} \rho_{23} \quad (16)$$

It follows that the centered covariance of  $U_1^2$  and  $U_2^2$  is

$$\text{Cov}(U_1^2, U_2^2) = 2 \rho_{12}^2$$

Consequently

$$G_h(x' - x) = \text{Cov}(Q_h(x), Q_h(x')) = \frac{2}{M^2} [\text{Cov}(Z_h(x), Z_h(x'))]^2 = \frac{2}{M^2} [C_h(x' - x)]^2$$

where  $C_h(l)$  is the covariance defined in (6) and expressed by (7) in terms of the GC  $K(h)$ .

#### Bessel Case $Z_1(x) = U(x) V(x)$

Consider a random function  $Z_1(x) = U(x) V(x)$ , where  $U(x)$  and  $V(x)$  are two independent Gaussian  $\mathcal{N}(0, 1)$  SRFs with the same correlogram  $\rho(h)$ . As  $U$  and  $V$  are independent, the calculation of  $G_h(x' - x)$  is based on (16).

If  $k = 0$ , we obtain:

$$\begin{aligned}
G_h(x' - x) = & 2\rho(x' - x)^2 + \rho(x' - x - h)^2 + \rho(x' - x + h)^2 + 3\rho(x' - x)^4 + \rho(x' - x - h)^4 + \rho(x' - x + h)^4 \\
& - 4\rho(x' - x)^2 \rho(x' - x - h)^2 - 4\rho(x' - x)^2 \rho(x' - x + h)^2 \\
& + 2\rho(h)^2 \rho(x' - x)^2 + \rho(x' - x - h)^2 \rho(x' - x + h)^2 \\
& - 4\rho(h) \rho(x' - x) \rho(x' - x - h) - 4\rho(h) \rho(x' - x) \rho(x' - x + h) \\
& + 2\rho(h)^2 \rho(x' - x - h) \rho(x' - x + h) + 2\rho(x' - x)^2 \rho(x' - x - h) \rho(x' - x + h)
\end{aligned}$$

### Gamma (chi-2) Case $Z_2(x) = U(x)^2$

Consider a random function  $Z_2(x) = U(x)^2$ , where  $U(x)$  is a Gaussian  $\mathcal{N}(0, 1)$  SRF with correlogram  $\rho(h)$ . The calculation of  $G_h(x' - x)$  calls for moments of order 8 of the SRF  $U$ . In fact only moments of the centered SRF  $H(x) = U(x)^2 - 1$  are needed. The expression of these moments is based on the following property:

If  $U_1, U_2, U_3, U_4$  are  $\mathcal{N}(0, 1)$  random variables, with correlation coefficients  $\rho_{ij}$ , and if the random vector  $(U_1, U_2, U_3, U_4)'$  is Gaussian, then the fourth-order moment of the centered square values  $H_i = U_i^2 - 1$ ,  $i = 1, 2, 3, 4$ , is

$$E[H_1 H_2 H_3 H_4] = 4(\rho_{12}^2 \rho_{34}^2 + \rho_{13}^2 \rho_{24}^2 + \rho_{14}^2 \rho_{23}^2) + 16(\rho_{12} \rho_{23} \rho_{34} \rho_{41} + \rho_{12} \rho_{34} \rho_{13} \rho_{24} + \rho_{23} \rho_{41} \rho_{13} \rho_{24})$$

Applying this relation to the case  $k = 0$ , one finds that:

$$\begin{aligned}
G_h(x' - x) = & 8 \left[ 2\rho(x' - x)^2 + \rho(x' - x - h)^2 + \rho(x' - x + h)^2 \right] \\
& + 6 \left[ \rho(x' - x - h)^4 + \rho(x' - x + h)^4 \right] \\
& + 16 \left[ \rho(h)^2 + \rho(x' - x)^2 \right] \left[ \rho(x' - x)^2 + \rho(x' - x - h) \rho(x' - x + h) \right] \\
& + 4 \left[ \rho(x' - x - h)^2 \rho(x' - x + h)^2 \right] \\
& - 24 \rho(x' - x)^2 \left[ \rho(x' - x - h)^2 + \rho(x' - x + h)^2 \right] \\
& - 32 \rho(h) \rho(x' - x) \left[ \rho(x' - x - h) + \rho(x' - x + h) \right]
\end{aligned}$$

### Lognormal Case $Z_3(x) = e^{U(x)}$

Consider a random function  $Z_3(x) = e^{U(x)}$ , where  $U(x)$  is a  $\mathcal{N}(0, 1)$  SRF with correlogram  $\rho(h)$ . The calculation of  $G_h(x' - x)$  is based on the following property:

If  $U_i$ ,  $i = 1, 2, \dots, p$ , are  $\mathcal{N}(0, 1)$  random variables, with correlation coefficients  $\rho_{ij}$ , and if the random vector  $(U_1, U_2, \dots, U_p)'$  is Gaussian, then

$$E \left[ \exp \left( \sum_i a_i U_i \right) \right] = \exp(\sigma^2 / 2) \quad \text{with} \quad \sigma^2 = \sum_i \sum_j a_i a_j \rho_{ij}$$

Using this relation, one gets in the case  $k = 0$ :

$$G_h(x' - x) = e^2 \left[ \begin{array}{l} \frac{1}{2} e^{2+4\rho(x'-x)} + \frac{1}{4} e^{2+4\rho(x'-x-h)} + \frac{1}{4} e^{2+4\rho(x'-x+h)} \\ - e^{1+\rho(h)+2\rho(x'-x)+2\rho(x'-x-h)} - e^{1+\rho(h)+2\rho(x'-x)+2\rho(x'-x+h)} \\ + e^{2\rho(h)+2\rho(x'-x)+\rho(x'-x-h)+\rho(x'-x+h)} - (e - e^{\rho(h)})^2 \end{array} \right]$$



## APPENDIX B

### ESTIMATION VARIANCE IN THE GAUSSIAN CASE

Consider the case of a Gaussian IRF- $k$  and of regularly located data. According to (11), (12), and (13), the estimation variance  $\text{Var}[\hat{\Gamma}(h) - \Gamma_R(h)]$  is the variance of estimation of the average value of the variable  $Q_h$  within  $D_h$  by the average of  $N_h$  regularly located data. The covariance of  $Q_h$  is  $G_h(x' - x) = \frac{2}{M^2} C_h(x' - x)^2$  according to (14). The variance of estimation is essentially linked with the irregular—that is, uneven—terms of lower degree of the covariance  $G_h$  in the vicinity of the origin (Matheron, 1965, pp. 192–208). Indeed, the even-degree terms have no influence on the variance, and among the other terms, those of lower degree cause the greater part of the variance, notably the lowest-degree term, known as the principal irregular term.

In the present case, for  $|x' - x| \ll h$ , the development of  $C_h(x' - x)$  at the origin is obtained by replacing  $K(x' - x + ph)$  by  $K(ph)$  in (7), except for the term corresponding to  $p = 0$ , which leads to

$$C_h(x' - x) \approx C_h(0) + \binom{2k+2}{k+1} [K(x' - x) - K(0)]$$

or equivalently

$$C_h(x' - x) \approx M [\Gamma(h) + K(x' - x) - K(0)]$$

It follows that the principal irregular term of  $G_h(x' - x)$  is the principal irregular term of

$$4\Gamma(h) [K(x' - x) - K(0)]$$

The estimation variance of  $\Gamma_R(h)$  (average value of  $Q_h(x)$ ) can be computed therefore, to a first approximation, as if  $Q_h$  had a variogram with a behavior near the origin equal to  $K(0) - K(x' - x)$  multiplied by  $4\Gamma(h)$ . The GC  $K(\cdot)$  is defined up to an even polynomial, but this is not important, as even terms bring no contribution to the estimation variance.

For 1D data at mesh  $d$ , we then have

$$\frac{\text{Var}[\hat{\Gamma}(h) - \Gamma_R(h)]}{\Gamma(h)^2} \approx \frac{4}{\Gamma(h)} \frac{\sigma_d^2}{N_h} \quad (17)$$

where  $\sigma_d^2$  is the estimation variance of the elementary mesh by its central value for a variable with a covariance equal to  $K(\cdot)$  near the origin, and where  $N_h$  is the number of available experimental increments of order  $k + 1$ .

For example, if a segment of length  $L$  is sampled by  $N = L / d$  points, and if  $h = jd$ ,  $\hat{\Gamma}(jd)$  can be computed from  $N_h = N - (k + 1)j$  increments. If  $K(x' - x)$  is of the form  $(-1)^{1+\lfloor\alpha/2\rfloor} b |x' - x|^\alpha$  with  $0 < \alpha < 2k + 2$  and  $b > 0$ , then one has

$$\Gamma(h) = (-1)^{1+\lfloor\alpha/2\rfloor} b B_\alpha |h|^\alpha$$

where  $B_\alpha$  (which depends on  $k$ ) is given by (8). And it is found to a first approximation (Matheron, 1965, pp. 205 and 82) that

$$\sigma_d^2 = (-1)^{1+\lfloor\alpha/2\rfloor} b T_\alpha d^\alpha \quad \text{with} \quad T_\alpha = -2 \sin\left(\frac{\alpha\pi}{2}\right) \frac{R_{1+\alpha}}{1+\alpha}$$

where  $R_\beta$  is the generalized Bernoulli number

$$R_\beta = \frac{\Gamma(1+\beta)}{\pi^\beta 2^{\beta-1}} \sum_{n=1}^{\infty} \frac{1}{n^\beta}$$

Here  $\Gamma(\cdot)$  denotes the Euler gamma function. In particular:

$$T_1 = -1/6$$

$$T_3 = 1/60$$

$$T_5 = -1/126$$

Hence the relative variance (17) is:

$$\frac{\text{Var}\left[\hat{\Gamma}(jd) - \Gamma_R(jd)\right]}{\Gamma(jd)^2} \simeq \frac{4}{N - (k+1)j} \frac{T_\alpha}{B_\alpha} \frac{1}{j^\alpha} \quad (18)$$

Similarly, if  $K(x' - x)$  is of the form  $(-1)^{m+1} b |x' - x|^{2m} \log |x' - x|$  near the origin, one has

$$\Gamma(h) = (-1)^{m+1} b B_{2m} |h|^{2m}$$

where the first  $B_{2m}$  values can be found in the expression of  $\Gamma(h)$  for a polynomial/logarithmic GC. And to a first approximation (Matheron, 1965, pp. 206 et 82)

$$\sigma_d^2 = (-1)^{1+m} b T'_{2m} d^{2m} \quad \text{with} \quad T'_{2m} = (-1)^{1+m} \frac{\pi}{1+2m} R_{1+2m}$$

where  $R_\beta$  is defined as above. In particular

$$T'_2 = 0.06090$$

$$T'_4 = -0.01597$$

$$T'_6 = 0.01208$$

Hence the expression (18) remains valid by taking  $\alpha = 2m$  and by replacing  $T$  by  $T'$  (their definitions differ by a multiplicative factor).

## APPENDIX C

### FLUCTUATION VARIANCE IN THE GAUSSIAN CASE

Consider a Gaussian IRF- $k$   $Z(x)$ . According to (14) and (15), the fluctuation variance of the regional GV of domain  $D$  is

$$\text{Var}[\Gamma_R(h) - \Gamma(h)] = \frac{2}{M^2 |D_h|^2} \int_{D_h} \int_{D_h} C_h(x' - x)^2 dx dx'$$

From a practical point of view, the double integral can be expressed as a simple integral using the change of variable  $u = x' - x$  (*Cauchy algorithm*):

$$\text{Var}[\Gamma_R(h) - \Gamma(h)] = \frac{4}{M^2 |D_h|^2} \int R_h(u) C_h(u)^2 du \quad (19)$$

where  $R_h$  is the geometrical covariogram of  $D_h$ , that is,  $R_h = 1_{D_h} * \tilde{1}_{D_h}$  if  $1_{D_h}$  denotes the indicator function of domain  $D_h$  and  $\tilde{1}_{D_h}$  denotes its transpose.

#### Behavior at Short Distances

Consider now the behavior of this variance for small values of  $h$ . If  $|h| \simeq 0$ , then (19) becomes, to a first approximation:

$$\text{Var}[\Gamma_R(h) - \Gamma(h)] \simeq \frac{4}{M^2 |D|^2} \int R(u) C_h(u)^2 du \quad (20)$$

where the geometric covariogram  $R$  of  $D$  replaces  $R_h$ .  $C_h$  is the covariance of the increment of order  $k+1$ , which is defined by (3). This increment is of the form  $\Delta_h^{k+1} Z(x) = \sum_{i=0}^{k+1} \lambda_i Z(x+ih)$

with  $\lambda_i = (-1)^{k+1+i} \binom{k+1}{i}$ . Therefore,  $C_h$  is of the form

$$C_h(u) = \sum_{i=0}^{k+1} \sum_{j=0}^{k+1} \lambda_i \lambda_j K(u + (j-i)h) \quad (21)$$

Let us separate the computation of the integral defined in (20) in two parts:

i)  $|u| > (k+1)|h|$

Suppose that  $K$  is regular enough to be locally expressed from its derivatives, except around 0 (this is not always the case, strictly speaking; an example is a spherical covariance around a

lag equal to the range; in such a case, it suffices to slightly regularize the covariance). So for  $|v| < |u|$  we have

$$K(u+v) \simeq \sum_{p=0}^{\infty} \frac{K^{(p)}(u)}{p!} v^p$$

Because  $|(j-i)h| < |u|$ , formula (21) becomes

$$C_h(u) \simeq \sum_{p=0}^{\infty} \frac{K^{(p)}(u)}{p!} \sum_{i=0}^{k+1} \sum_{j=0}^{k+1} \lambda_i \lambda_j (j-i)^p |h|^p$$

(the derivatives at  $u$  are taken along the orientation of vector  $h$ ). If  $p$  is odd, the double sum on  $i$  and  $j$  is null due to symmetry. If  $p$  is even, this double sum coincides with the variance of  $\Delta_h^{k+1} Z(x)$  for a covariance  $|h|^p$ , with the exception that  $|h|^p$  is not necessarily a GC. If  $p \leq 2k$ , it is a GC (up to the sign), and the associated variance is null. The first non-zero term is then associated with  $p = 2k + 2$ , so that

$$C_h(u) \simeq \tau |h|^{2k+2} K^{(2k+2)}(u)$$

with

$$\tau = \frac{1}{(2k+2)!} \sum_{i=0}^{k+1} \sum_{j=0}^{k+1} \lambda_i \lambda_j (j-i)^{2k+2}$$

It follows that the part of (20) corresponding to the integration domain  $|u| > (k+1)|h|$  is, to a first approximation, of the form

$$A' |h|^{4k+4}$$

ii)  $|u| \leq (k+1)|h|$

The behavior of the GC in the vicinity of the origin plays the main role in the calculation of (20). Suppose that the principal irregular term of  $K(h)$  is  $(-1)^{1+\lfloor \alpha/2 \rfloor} b |h|^\alpha$ . Then (21) becomes:

$$C_h(u) \simeq (-1)^{1+\lfloor \alpha/2 \rfloor} b |h|^\alpha \sum_{i=0}^{k+1} \sum_{j=0}^{k+1} \lambda_i \lambda_j \left| (j-i) \frac{h}{|h|} + \frac{u}{|h|} \right|^\alpha$$

Since  $h$  is small, by substituting  $v = u / |h|$  one finds:

$$\int_{|u| \leq (k+1)|h|} R(u) C_h(u)^2 du \simeq R(0) b^2 |h|^{2\alpha+n} \int_{|v| \leq k+1} \left[ \sum_{i=0}^{k+1} \sum_{j=0}^{k+1} \lambda_i \lambda_j \left| (j-i) \frac{h}{|h|} + v \right|^\alpha \right]^2 dv$$

where  $n$  is the space dimension. Hence the part of (20) corresponding to the integration domain  $|u| \leq (k+1)|h|$  is, to a first approximation, of the form:

$$B' |h|^{2\alpha+n}$$

As a consequence of (i) and (ii), since a behavior in  $(-1)^{1+\lfloor\alpha/2\rfloor} b |h|^\alpha$  in the vicinity of the origin is considered for  $K(h)$  (behavior which is the same, up to a multiplicative factor, for the GV), it is found that for small  $h$  values the relative fluctuation variance takes the form:

$$S_F^2(h) = \frac{\text{Var}[(\Gamma_R(h) - \Gamma(h))]}{\Gamma(h)^2} \simeq A|h|^{4k+4-2\alpha} + B|h|^n$$

### Explicit Calculation for Some GCs in the 1D Case

The explicit calculation of (19) is simple in the 1D case. Consider that the domain  $D$  is a segment of length  $L$ .  $D_h$  is then a segment of length  $L_h = L - (k+1)h$ , and its geometrical covariogram is  $R_h(u) = \sup(L_h - |u|, 0)$ . Formula (19) then becomes

$$\text{Var}[(\Gamma_R(h) - \Gamma(h))] = \frac{4}{M^2 |L_h|^2} \int_0^{L_h} (L_h - u) C_h(u)^2 du \quad (20)$$

The relative variance  $S_F^2(h) = \text{Var}[(\Gamma_R(h) - \Gamma(h))] / \Gamma(h)^2$  is given below for several GC models. The notations  $h$  and  $u$  stand for  $|h|$  and  $|u|$ .

i)  $k = 0$   $K(h) = -h$

$$C_h(u) = \begin{cases} 2(h-u) & \text{if } u \leq h \\ 0 & \text{if } u \geq h \end{cases}$$

$$\Gamma(h) = h$$

$$S_F^2(h) = \begin{cases} \frac{4}{3} \frac{h}{L-h} - \frac{1}{3} \frac{h^2}{(L-h)^2} & \text{if } 0 \leq h \leq \frac{L}{2} \\ 2 - \frac{4}{3} \frac{L-h}{h} + \frac{1}{3} \frac{(L-h)^2}{L^2} & \text{if } \frac{L}{2} \leq h \leq L \end{cases}$$

In particular:  $h \rightarrow 0$ :  $S_F^2(h) \simeq \frac{4}{3} \frac{h}{L}$

$h = \frac{L}{2}$ :  $S_F^2(h) = 1$

$h \rightarrow L$ :  $S_F^2(h) \simeq 2 - \frac{4}{3} \left(1 - \frac{h}{L}\right)$

ii)  $k = 1$   $K(h) = -h$

$$C_h(u) = \begin{cases} 2(2h - 3u) & \text{if } u \leq h \\ 2(-2h + u) & \text{if } h \leq u \leq 2h \\ 0 & \text{if } u \geq 2h \end{cases}$$

$$\Gamma(h) = \frac{2}{3}h$$

$$S_F^2(h) = \begin{cases} \frac{4}{3}r - \frac{2}{3}r^2 & \text{if } 0 \leq h \leq \frac{L}{4} \\ \frac{2}{3}r^2 - \frac{4}{3}r + 2 - \frac{2}{3}r^{-1} + \frac{1}{12}r^{-2} & \text{if } \frac{L}{4} \leq h \leq \frac{L}{3} \\ 2 - 2r^{-1} + \frac{3}{4}r^{-2} & \text{if } \frac{L}{3} \leq h \leq \frac{L}{2} \end{cases} \quad \text{with} \quad r = \frac{h}{L - 2h}$$

$$\begin{aligned} \text{In particular: } h \rightarrow 0: \quad S_F^2(h) &\simeq \frac{4}{3} \frac{h}{L} \\ h = \frac{L}{4}: \quad S_F^2(h) &= \frac{1}{2} \\ h \rightarrow \frac{L}{2}: \quad S_F^2(h) &\simeq 2 - 4 \left(1 - \frac{2h}{L}\right) \end{aligned}$$

At short distances, the precision remains the same as for  $k = 0$ .

iii)  $k = 1$   $K(h) = h^3$

$$C_h(u) = \begin{cases} 2(4h^3 - 6hu^2 + 3u^3) & \text{if } u \leq h \\ 2(8h^3 - 12h^2u + 6hu^2 - u^3) & \text{if } h \leq u \leq 2h \\ 0 & \text{if } u \geq 2h \end{cases}$$

$$\Gamma(h) = \frac{4}{3}h^3$$

$$S_F^2(h) = \begin{cases} \frac{151}{70}r - \frac{103}{140}r^2 & \text{if } 0 \leq h \leq \frac{L}{4} \\ \frac{57}{140}r^2 - \frac{169}{70}r + 8 - 8r^{-1} + 5r^{-2} - 2r^{-3} + \frac{1}{2}r^{-4} - \frac{1}{14}r^{-5} + \frac{1}{224}r^{-6} & \text{if } \frac{L}{4} \leq h \leq \frac{L}{3} \\ 2 - r^{-2} + \frac{3}{10}r^{-3} + \frac{3}{10}r^{-4} - \frac{3}{14}r^{-5} + \frac{9}{224}r^{-6} & \text{if } \frac{L}{3} \leq h \leq \frac{L}{2} \end{cases}$$

with  $r = \frac{h}{L - 2h}$

$$\begin{aligned} \text{In particular: } h \rightarrow 0: \quad S_F^2(h) &\simeq \frac{151}{70} \frac{h}{L} \\ h = \frac{L}{4}: \quad S_F^2(h) &= \frac{501}{560} \\ h \rightarrow \frac{L}{2}: \quad S_F^2(h) &\simeq 2 - 4 \left(1 - \frac{2h}{L}\right)^2 \end{aligned}$$

At short distances, the precision is only slightly less than for a linear covariance.

$$\text{iv) } k=0 \quad K(h) = e^{-h/a}$$

$$C_h(u) = \begin{cases} 2e^{-u/a} - e^{-h/a} [e^{u/a} + e^{-u/a}] & \text{if } 0 \leq u \leq h \\ e^{-u/a} [2 - e^{h/a} - e^{-h/a}] & \text{if } u \geq h \end{cases}$$

$$\Gamma(h) = 1 - e^{-h/a}$$

$$S_F^2(h) = \frac{A(h)}{(L-h)^2 (1 - e^{-h/a})^2}$$

with

$$A(h) = \begin{cases} -\frac{3}{4}a^2 + \frac{5}{2}aL - 3ah + (a^2 - 2aL + 2ah - 4Lh + 6h^2)e^{-h/a} \\ \quad + (\frac{1}{2}a^2 - 2aL + 4ah + 2Lh - 3h^2)e^{-2h/a} \\ \quad + (a^2 - 2aL + 4ah)(\frac{1}{4}e^{-4h/a} - e^{-3h/a}) \\ \quad + a(1 - \frac{1}{2}e^{-h/a} - \frac{1}{2}e^{h/a})^2 (ae^{-2(L-h)/a} + (2L - a - 4h)e^{-2h/a}) & \text{if } 0 \leq h \leq \frac{1}{2}L \\ 2a(L-h) - a^2 - (2(L-h)^2 + 2a(L-h) - a^2)e^{-h/a} \\ \quad + ((L-h)^2 - \frac{1}{2}a^2)e^{-2h/a} \\ \quad + a^2(e^{-(2L-2h)/a} - e^{-(2L-h)/a} + \frac{1}{4}e^{-2L/a} + \frac{1}{4}e^{-(4h-2L)/a}) & \text{if } \frac{1}{2}L \leq h \leq L \end{cases}$$

From Taylor expansions at order 3 near 0 or  $L$ , we obtain:

$$h \rightarrow 0: \quad S_F^2(h) \approx \frac{4}{3} \frac{h}{L}$$

$$h \rightarrow L: \quad S_F^2(h) \approx 2 - \frac{4}{3} \frac{L-h}{a(1 - e^{-L/a})}$$

The value of  $S_F^2(L/2)$  decreases from 1 to 0 when  $L/a$  increases from 0 (linear variogram) to  $\infty$  (pure nugget effect). It is about 0.8616 when  $L = a$ .

## APPENDIX D

### Program MARKO

#### Computation of the Fluctuation Variance and of the Estimation Variance of the Generalized Variogram in the Gaussian Case

```
C PROGRAMME MARKO
C
C
C
C
C   Objet
C   Calcul de la variance de fluctuation et de la variance
C   d'estimation du variogramme generalise regional d'un rectangle
C   sous les conditions suivantes :
C       - discretisation du rectangle par NDX0 * NDY0 points;
C       - reconnaissance par NPX0 * NPY0 points a maille reguliere
C         (dispositif ferme);
C       - loi gaussienne.
C
C   NDX0, NDY0, NPX0 et NPY0 doivent etre de la forme :
C       - NDX0 = 1 + LX*NX*(KDEG+1)      NDY0 = 1 + LY*NY*(KDEG+1)
C       - NPX0 = 1 +   NX*(KDEG+1)      NPY0 = 1 +   NY*(KDEG+1)
C
C   L'acquisition des parametres limite le calcul a deux cas :
C       - segment 1-D :  NDX0=ND0  NDY0=1  NPX0=NP0  NPY0=1
C       - carre 2-D :   NDX0 = NDY0 = ND0  NPX0 = NPY0 = NP0
C
C   Parametres
C       - NDIM : Dimension de l'espace (1 ou 2)
C       - KDEG : degre k du variogramme generalise (0 a 3)
C               (k=0 pour un variogramme ordinaire)
C       - ITYPE : type de covariance generalisee (1 a 5)
C       - ALPHA : portee, ou parametre Alpha du modele h**Alpha
C                 ou h**Alpha*Log(h) si Alpha pair
C       - ND0 : discretisation du segment ou du carre
C       - NP0 : reseau des points experimentaux
C
C   Notations
C       COVG : covariance generalisee K(h)
C       COVQ : covariance quadratique G(x-y;h) (c'est la covariance
C             de la F.A. Q(x;h) = carre normalise de
C             l'accroissement d'ordre KDEG+1 pour le pas h)
C
C
C   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C   DIMENSION U(72722)
C   INTEGER ADCOVG,ADCOVQ
C   CHARACTER*24 FICIN,FICOUT
C
C   La dimension de U permet a 2-D d'aller jusqu'a ND0=121
C   DATA NDIMU/72722/
C
C
```



```

1 WRITE(3,3001)
3001 FORMAT(' Fichier en entree >', $)
READ(1,1001) FICIN
1001 FORMAT(A24)
IF(FICIN.NE.' ') THEN
OPEN(10, FILE=FICIN, STATUS='OLD', ERR=1)
ENDIF
2 WRITE(3,3002)
3002 FORMAT(' Fichier en sortie >', $)
READ(1,1002) FICOUT
1002 FORMAT(A24)
IF(FICOUT.NE.' ') THEN
OPEN(20, FILE=FICOUT, STATUS='NEW', CARRIAGECONTROL='LIST', ERR=2)
ENDIF
10 IF(FICIN.EQ.' ') THEN
WRITE(3,3011)
3011 FORMAT(' NDIM, KDEG, ITYPE, ALPHA, ND0, NP0 >', $)
READ(1, *, END=99) NDIM, KDEG, ITYPE, ALPHA, ND0, NP0
ELSE
READ(10, *, END=99) NDIM, KDEG, ITYPE, ALPHA, ND0, NP0
ENDIF
NDX0=ND0
NDY0=1
IF(NDIM.GT.1) NDY0=ND0
NPX0=NP0
NPY0=1
IF(NDIM.GT.1) NPY0=NP0
KHXMA=NDX0-1
KHYMA=NDY0-1
ADCOVG=1
ADCOVQ=ADCOVG+NDX0*NDY0
LASTAD=ADCOVQ+(2*NDX0-1)*(2*NDY0-1)-1
IF(LASTAD.GT.NDIMU) GO TO 90
CALL MARKO(U(ADCOVG), U(ADCOVQ), NDIM, KDEG, ITYPE, ALPHA, NDX0, NDY0,
& NPX0, NPY0, KHXMA, KHYMA, FICOUT)
GO TO 10
C
90 WRITE(3,3090)
3090 FORMAT('1*** U est trop petit.')
C
99 STOP
END
SUBROUTINE MARKO(COVG, COVQ, NDIM, KDEG, ITYPE, ALPHA, NDX0, NDY0,
& NPX0, NPY0, KHXMA, KHYMA, FICOUT)
C
C
IMPLICIT DOUBLE PRECISION (A-H, O-Z)
DIMENSION COVG(0:KHXMA, 0:KHYMA), COVQ(-KHXMA:KHXMA, -KHYMA:KHYMA)
DIMENSION SCHEMA(5)
CHARACTER*24 FICOUT
INTEGER DELX, DELY
LOGICAL SKIP
C
DATA SCHEMA/8Hspheriq., 8Hexpon. , 8Hcubique , 8Hgaussien,
& 8Hh**Alpha/
C
C
KLOI=0
IF(KDEG.EQ.0) THEN
MK=2
ELSEIF(KDEG.EQ.1) THEN

```

```

        MK=6
    ELSEIF (KDEG.EQ.2) THEN
        MK=20
    ELSEIF (KDEG.EQ.3) THEN
        MK=70
    ENDIF
C
    IF (FICOUT.EQ.' ') THEN
        WRITE (3,3101) NDIM,KDEG,SCHEMA (ITYPE),ALPHA,NDX0,NPX0
3101    FORMAT (1H1,I1,'-D',5X,'k =',I2,5X,'Schema ',A8,5X,
&          'Alpha =',F5.1,7X,'ND0 =',I4,5X,'NP0 =',I4)
        WRITE (3,3102)
3102    FORMAT (1H0/1H ,29X,'Fluctuations',20X,'Estimation'/
&          17H0 h          Gamma ,
&          2 (32H          Var          Var rel          Sig rel)/1H )
        ELSE
            WRITE (20,3103) NDIM,KDEG,SCHEMA (ITYPE),ALPHA,NDX0,NPX0
3103    FORMAT (/1H ,I1,'-D',5X,'k =',I2,5X,'Schema ',A8,5X,
&          'Alpha =',F5.1,7X,'ND0 =',I4,5X,'NP0 =',I4)
            WRITE (20,3104)
3104    FORMAT (/1H , ' H          Fluctu          Estim')
            WRITE (3,3105) NDIM,KDEG,SCHEMA (ITYPE),ALPHA,NDX0,NPX0
3105    FORMAT (1H ,I1,'-D',5X,'k =',I2,5X,'Schema ',A8,5X,
&          'Alpha =',F5.1,7X,'ND0 =',I4,5X,'NP0 =',I4)
        ENDIF
C
C
C          Calcul des valeurs utiles de la covariance de la gaussienne
C
C
        DO 1 KHY=0,NDY0-1
        DO 1 KHX=0,NDX0-1
            H=DSQRT (DFLOAT (KHX**2+KHY**2)) / (NDX0-1)
            COVG (KHX,KHY)=COVGEN (H,ITYPE,ALPHA)
1 CONTINUE
C
C
C          Boucle sur la distance de calcul du variogramme (direction X)
C
C
        KHMAX=(NDX0-1)/(KDEG+1)
        HMAX=1./DFLOAT (KDEG+1)
        IXPAS=1
        IF (NPX0.GT.1) IXPAS=(NDX0-1)/(NPX0-1)
        IYPAS=1
        IF (NPY0.GT.1) IYPAS=(NDY0-1)/(NPY0-1)
        SKIP=.FALSE.
C
        DO 90 KH=IXPAS,KHMAX,IXPAS
C
            H=DFLOAT (KH)/DFLOAT (NDX0-1)
C
C          Elimination des distances "tordues" lorsque NDX0 est grand
C
            IF (FICOUT.NE.' ') GO TO 10
            IF (NDIM.EQ.2) GO TO 10
            IF (KDEG.GE.2) GO TO 10
            IF (H.LE.0.1.OR.H.GE.HMAX-0.1) GO TO 10
            PAS=0.1/DFLOAT (KDEG+1)
            D=DMOD (H,PAS)
            IF (D.LT.0.001.OR.D.GT.PAS-0.001) GO TO 10

```

```

IF (.NOT.SKIP) WRITE (3,3010)
3010  FORMAT (1H )
      SKIP=.TRUE.
      GO TO 90
C
      10  SKIP=.FALSE.
          NDX=NDX0 - (KDEG+1) *KH
          NDY=NDY0
          NPX=NPX0 - (KDEG+1) *KH/IXPAS
          NPY=NPY0
C
C      Calcul des valeurs utiles de la covariance quadratique
C      (pour la valeur h)
C
          DO 15 DELY=-NDY+1,NDY-1
          DO 15 DELX=-NDX+1,NDX-1
C
          IF (KDEG.EQ.0) THEN
              G = 2.*COVG ( IABS (DELX) , IABS (DELY) )
&              - COVG ( IABS (DELX+KH) , IABS (DELY) )
&              - COVG ( IABS (DELX-KH) , IABS (DELY) )
C
          ELSEIF (KDEG.EQ.1) THEN
              G = 6.*COVG ( IABS (DELX) , IABS (DELY) )
&              - 4.*COVG ( IABS (DELX+KH) , IABS (DELY) )
&              - 4.*COVG ( IABS (DELX-KH) , IABS (DELY) )
&              + COVG ( IABS (DELX+2*KH) , IABS (DELY) )
&              + COVG ( IABS (DELX-2*KH) , IABS (DELY) )
C
          ELSEIF (KDEG.EQ.2) THEN
              G = 20.*COVG ( IABS (DELX) , IABS (DELY) )
&              -15.*COVG ( IABS (DELX+KH) , IABS (DELY) )
&              -15.*COVG ( IABS (DELX-KH) , IABS (DELY) )
&              + 6.*COVG ( IABS (DELX+2*KH) , IABS (DELY) )
&              + 6.*COVG ( IABS (DELX-2*KH) , IABS (DELY) )
&              - COVG ( IABS (DELX+3*KH) , IABS (DELY) )
&              - COVG ( IABS (DELX-3*KH) , IABS (DELY) )
C
          ELSEIF (KDEG.EQ.3) THEN
              G = 70.*COVG ( IABS (DELX) , IABS (DELY) )
&              -56.*COVG ( IABS (DELX+KH) , IABS (DELY) )
&              -56.*COVG ( IABS (DELX-KH) , IABS (DELY) )
&              +28.*COVG ( IABS (DELX+2*KH) , IABS (DELY) )
&              +28.*COVG ( IABS (DELX-2*KH) , IABS (DELY) )
&              - 8.*COVG ( IABS (DELX+3*KH) , IABS (DELY) )
&              - 8.*COVG ( IABS (DELX-3*KH) , IABS (DELY) )
&              + COVG ( IABS (DELX+4*KH) , IABS (DELY) )
&              + COVG ( IABS (DELX-4*KH) , IABS (DELY) )
C
          ENDIF
C
          COVQ (DELX,DELY)=2.*G**2/MK**2
C
      15  CONTINUE
C
      Double somme des G(ID-JD;KH) , ID,JD decrivant le domaine Vh
C
      GDD=0.
C
      La boucle 22 est la traduction optimisee du calcul suivant :
C
      DO 22 IDY=1,NDY
C
      DO 22 IDX=1,NDX

```

```

C      DO 22 JDY=1,NDY
C      DO 22 JDX=1,NDX
C          GDD=GDD+COVQ(JDX-IDX,JDY-IDY)
C 22    CONTINUE
C          DO 22 DELY=-NDY+1,NDY-1
C              NY=NDY-IABS(DELY)
C              GGG=0.
C              DO 21 DELX=-NDX+1,NDX-1
C                  NX=NDX-IABS(DELX)
C                  GGG=GGG+NX*COVQ(DELX,DELY)
C 21    CONTINUE
C          GDD=GDD+NY*GGG
C 22    CONTINUE
C          GDD=GDD/((NDX*NDY)**2)
C
C      Double somme des G(IP-JP;KH), IP,JP decrivant les points exp.
C
C          GPP=GDD
C          IF(NPX0.EQ.NDX0.AND.NPY0.EQ.NDY0) GO TO 40
C          GPP=0.
C      La boucle 32 est la traduction optimisee du calcul suivant :
C      DO 32 IPY=1,NDY,IYPAS
C      DO 32 IPX=1,NDX,IXPAS
C      DO 32 JPY=1,NDY,IYPAS
C      DO 32 JPX=1,NDX,IXPAS
C          GDD=GDD+COVQ(JPX-IPX,JPY-IPY)
C 32    CONTINUE
C          DO 32 DELY=-NDY+1,NDY-1,IYPAS
C              NY=1+(NDY-1)/IYPAS-IABS(DELY)/IYPAS
C              GGG=0.
C              DO 31 DELX=-NDX+1,NDX-1,IXPAS
C                  NX=1+(NDX-1)/IXPAS-IABS(DELX)/IXPAS
C                  GGG=GGG+NX*COVQ(DELX,DELY)
C 31    CONTINUE
C          GPP=GPP+NY*GGG
C 32    CONTINUE
C          GPP=GPP/((NPX*NPY)**2)
C
C      Double somme des G(ID-IP;KH)
C
C 40    GDP=GDD
C          IF(NPX0.EQ.NDX0.AND.NPY0.EQ.NDY0) GO TO 50
C          GDP=0.
C      La boucle 42 est la traduction optimisee du calcul suivant :
C      DO 42 IDY=1,NDY
C      DO 42 IDX=1,NDX
C      DO 42 IPY=1,NDY,IYPAS
C      DO 42 IPX=1,NDX,IXPAS
C          GDP=GDP+COVQ(IDX-IPX,IDY-IPY)
C 42    CONTINUE
C          DO 42 DELY=-NDY+1,NDY-1
C              NY=1+(NDY-1-IABS(DELY))/IYPAS
C              GGG=0.
C              DO 41 DELX=-NDX+1,NDX-1
C                  NX=1+(NDX-1-IABS(DELX))/IXPAS
C                  GGG=GGG+NX*COVQ(DELX,DELY)
C 41    CONTINUE
C          GDP=GDP+NY*GGG
C 42    CONTINUE
C          GDP=GDP/(NDX*NDY*NPX*NPY)
C

```

```

C      Calcul du variogramme et des covariances
C
50     IF(KDEG.EQ.0) THEN
        GAM=COVG(0,0) - COVG( KH,0)
    ELSEIF(KDEG.EQ.1) THEN
        GAM=COVG(0,0) -4. *COVG( KH,0)/3. + COVG(2*KH,0)/3.
    ELSEIF(KDEG.EQ.2) THEN
        GAM=COVG(0,0) -1.5*COVG( KH,0) +0.6*COVG(2*KH,0)
&      -0.1*COVG(3*KH,0)
    ELSEIF(KDEG.EQ.3) THEN
        GAM=COVG(0,0) -1.6*COVG( KH,0) +0.8*COVG(2*KH,0)
&      -8. *COVG(3*KH,0)/35.+ COVG(4*KH,0)/35.
    ENDIF
    GAM2=GAM**2
    VARFLU=GDD
    SIGFLU=DSQRT(VARFLU)
    VAREST=GDD+GPP-2.*GDP
    IF(VAREST.LT.0.) VAREST=0.
    SIGEST=DSQRT(VAREST)
    IF(FICOUT.EQ.' ') THEN
        WRITE(3,3061) H,GAM,VARFLU,VARFLU/GAM2,SIGFLU/GAM,
&      VAREST,VAREST/GAM2,SIGEST/GAM
3061    FORMAT(1H ,F5.3,F10.3,1X,2(1X,3F10.3,1X))
    ELSE
        WRITE(20,3062) H,SIGFLU/GAM,SIGEST/GAM
3062    FORMAT(1H ,F5.3,2F8.4)
    ENDIF
C
90     CONTINUE
C
C
    RETURN
    END
    DOUBLE PRECISION FUNCTION COVGEN(H,ITYPE,ALPHA)
C
C
C      Covariance generalisee nulle en 0
C
C
    IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C
    GO TO (10,20,30,40,50),ITYPE
C
C      Modele spherique
C
10    IF(H.LT.ALPHA) THEN
        R=H/ALPHA
        GAMMA=1.5*R-0.5*R**3
    ELSE
        GAMMA=1.
    ENDIF
    GO TO 90
C
C      Modele exponentiel
C
20    R=H/ALPHA
    GAMMA=1.-DEXP(-R)
    GO TO 90
C
C      Modele cubique

```

```

C
30 IF (H.LT.ALPHA) THEN
    R=H/ALPHA
    R2=R**2
    GAMMA=R2*(7.-R*(8.75+R2*(-3.5+0.75*R2)))
ELSE
    GAMMA=1.
ENDIF
GO TO 90

C
C   Modele gaussien
C
40 R=H/ALPHA
    GAMMA=1.-DEXP(-0.5*R**2)
GO TO 90

C
C   Modele en h**Alpha, ou en h**Alpha*Log(h) si Alpha est pair
C
50 IF (H.EQ.0.) THEN
    GAMMA=0.
ELSE
    N=(ALPHA+0.0001)/2.
    IF (MOD(N,2).EQ.0) THEN
        SIGNE=+1.
    ELSE
        SIGNE=-1.
    ENDIF
    IF (DABS(ALPHA-2.*N).LT.0.0001) THEN
        GAMMA=SIGNE*H**(2*N)*DLOG(H)
    ELSE
        GAMMA=SIGNE*H**ALPHA
    ENDIF
ENDIF
GO TO 90

C
90 COVGEN=-GAMMA

C
RETURN
END

```

## APPENDIX E

### Program MARCO

#### Computation of the Fluctuation Variance and of the Estimation Variance of the Variogram in the Gaussian and Non-Gaussian Cases

```
C PROGRAMME MARCO
C
C
C OBJET
C   CALCUL DE LA VARIANCE DE FLUCTUATION ET DE LA VARIANCE
C   D'ESTIMATION DU VARIOGRAMME REGIONAL D'UN RECTANGLE
C   SOUS LES CONDITIONS SUIVANTES :
C     - DISCRETISATION DU RECTANGLE PAR NDX0 * NDY0 POINTS;
C     - RECONNAISSANCE PAR NPX0 * NPY0 POINTS A MAILLE REGULIERE
C       (DISPOSITIF FERME);
C     - LOI GAUSSIENNE, GAMMA, BESSEL, OU LOGNORMALE (IL S'AGIT
C       DE CAS PARTICULIERS, OBTENUS A PARTIR DE VARIABLES
C       GAUSSIENNES);
C     - SAUF DANS LE CAS D'UNE LOI GAUSSIENNE, VARIOGRAMME LIMITE
C       AU MODELE EXPONENTIEL (IMPOSE ITYPE=2, OU ITYPE=8 POUR
C       L'APPROXIMATION LOGNORMALE).
C
C   NDX0, NDY0, NPX0 ET NPY0 DOIVENT ETRE DE LA FORME :
C     - NDX0 = 1 + LX*NX           NDY0 = 1 + LY*NY
C     - NPX0 = 1 +   NX           NPY0 = 1 +   NY
C
C   L'ACQUISITION DES PARAMETRES LIMITE LE CALCUL A 2 CAS :
C     - SEGMENT 1-D :  NDX0=ND0  NDY0=1  NPX0=NP0  NPY0=1
C     - CARRE 2-D :  NDX0 = NDY0 = ND0  NPX0 = NPY0 = NP0
C
C   PARAMETRES
C     - NDIM : DIMENSION DE L'ESPACE (1 OU 2)
C     - KLOI : TYPE DE LOI (1 A 4)
C     - ITYPE : TYPE DE COVARIANCE OU DE VARIOGRAMME (1 A 7)
C     - ALPHA : PORTEE, OU PARAMETRE ALPHA DU MODELE H**ALPHA
C     - ND0 : DISCRETISATION DU SEGMENT OU DU CARRE
C     - NP0 : RESEAU DES POINTS EXPERIMENTAUX
C
C   NOTATIONS
C     COVG : COVARIANCE GENERALISEE D'ORDRE 0 K(H)
C           (=COVARIANCE ORDINAIRE OU -VARIOGRAMME)
C     COVQ : COVARIANCE QUADRATIQUE G(X-Y;H)
C           (=COVARIANCE DE LA F.A. Q(X) = (Z(X+H)-Z(X))**2 )
C
C   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C   DIMENSION U(72722)
C   INTEGER ADCOVG,ADCOVQ
C
C   LA DIMENSION DE U PERMET A 2-D D'ALLER JUSQU'A ND0=121
C   DATA NDIMU/72722/
C
C
```

```

1 READ (1, *, END=99) NDIM, KLOI, ITYPE, ALPHA, ND0, NP0
  IF (KLOI.EQ.0.AND.ITYPE.LE.5) GO TO 2
  IF (KLOI.EQ.0.AND.ITYPE.EQ.6.AND.NDIM.EQ.1) GO TO 2
  IF (KLOI.EQ.1.AND.ITYPE.EQ.2) GO TO 2
  IF (KLOI.EQ.2.AND.ITYPE.EQ.2) GO TO 2
  IF (KLOI.EQ.3.AND.ITYPE.EQ.2.AND.NDIM.EQ.1.AND.ALPHA.GE.1.) GO TO 2
  IF (KLOI.EQ.3.AND.ITYPE.EQ.8) GO TO 2
  GO TO 1
C
2 NDX0=ND0
  NDY0=1
  IF (NDIM.GT.1) NDY0=ND0
  NPX0=NP0
  NPY0=1
  IF (NDIM.GT.1) NPY0=NP0
  KHXMA=NDX0-1
  KHYMA=NDY0-1
  ADCOVG=1
  ADCOVQ=ADCOVG+NDX0*NDY0
  LASTAD=ADCOVQ+(2*NDX0-1)*(2*NDY0-1)-1
  IF (LASTAD.GT.NDIMU) GO TO 90
  CALL MARCO (U (ADCOVG), U (ADCOVQ), NDIM, KLOI, ITYPE, ALPHA, NDX0, NDY0,
& NPX0, NPY0, KHXMA, KHYMA)
  GO TO 1
C
90 WRITE (3, 300)
300 FORMAT ('1*** U TROP PETIT')
C
99 STOP
  END
  SUBROUTINE MARCO (COVG, COVQ, NDIM, KLOI, ITYPE, ALPHA, NDX0, NDY0,
& NPX0, NPY0, KHXMA, KHYMA)
C
C
  IMPLICIT DOUBLE PRECISION (A-H, O-Z)
  DIMENSION COVG (0:KHXMA, 0:KHYMA), COVQ (-KHXMA:KHXMA, -KHYMA:KHYMA)
  DIMENSION ALOI (0:3), SCHEMA (8)
  INTEGER DELX, DELY
  LOGICAL SKIP
C
  DATA ALOI /8HGAUSS, 8HGAMMA, 8HBESSEL, 8HLOGN. /
  DATA SCHEMA/8HSPHERIQ., 8HEXPON., 8HCUBIQUE, 8HGAUSSIEN,
& 8HH**ALPHA, 8HTRIANGLE, 8HMIXTE, 8HLOG.MIX./
C
C
  KDEG=0
  MK=2
C
  WRITE (3, 300) NDIM, ALOI (KLOI), SCHEMA (ITYPE), ALPHA, NDX0, NPX0
300 FORMAT (/1H, I1, '-D', 5X, 'LOI ', A6, 5X, 'SCHEMA ', A8, 5X, 'A =', F6.2,
& 5X, 'ND0 =', I4, 5X, 'NP0 =', I4)
  WRITE (3, 301)
301 FORMAT (/1H, ' H Fluctu Estim')
C
C
  PARAMETRES DU VARIOGRAMME DE LA VARIABLE GAUSSIENNE AUXILIAIRE
  (CF. COMMENTAIRES DE LA BOUCLE 15)
C
C
  IF (KLOI.EQ.0) THEN
    ITYPE1=ITYPE

```



```

        ALPHA1=ALPHA
ELSEIF (KLOI.EQ.1) THEN
        ITYPE1=2
        ALPHA1=2.*ALPHA
ELSEIF (KLOI.EQ.2) THEN
        ITYPE1=2
        ALPHA1=2.*ALPHA
ELSEIF (KLOI.EQ.3) THEN
        IF (ITYPE.EQ.2) ITYPE1=6
        IF (ITYPE.EQ.8) ITYPE1=7
        ALPHA1=ALPHA
ENDIF
C
C
C   CALCUL DES VALEURS UTILES DE LA COVARIANCE DE LA GAUSSIENNE
C
C
DO 1 KHY=0,NDY0-1
DO 1 KHX=0,NDX0-1
        H=DSQRT (DFLOAT (KHX**2+KHY**2)) / (NDX0-1)
        COVG (KHX, KHY) =COVGEN (H, ITYPE1, ALPHA1)
1 CONTINUE
C
C
C   BOUCLE SUR LA DISTANCE DE CALCUL DU VARIOGRAMME (DIRECTION X)
C
C
        KHMAX=NDX0-1
        HMAX=1.
        IXPAS=1
        IF (NPX0.GT.1) IXPAS= (NDX0-1) / (NPX0-1)
        IYPAS=1
        IF (NPY0.GT.1) IYPAS= (NDY0-1) / (NPY0-1)
        SKIP=.FALSE.
C
DO 90 KH=IXPAS, KHMAX, IXPAS
C
        H=DFLOAT (KH) /DFLOAT (NDX0-1)
C
        ELIMINATION DES DISTANCES "TORDUES" LORSQUE NDX0 EST GRAND
C
        IF (NDIM.EQ.1) GO TO 10
        IF (NDIM.EQ.2) GO TO 10
        IF (H.LE.0.1.OR.H.GE.HMAX-0.1) GO TO 10
        PAS=0.1
        D=DMOD (H, PAS)
        IF (D.LT.0.001.OR.D.GT.PAS-0.001) GO TO 10
        IF (.NOT.SKIP) WRITE (3,310)
310   FORMAT (1H )
        SKIP=.TRUE.
        GO TO 90
C
10   SKIP=.FALSE.
        NDX=NDX0-KH
        NDY=NDY0
        NPX=NPX0-KH/IXPAS
        NPY=NPY0
C
C   CALCUL DES VALEURS UTILES DE LA COVARIANCE QUADRATIQUE
C   DE LA VARIABLE NON GAUSSIENNE (POUR LA VALEUR H)
C

```

```

DO 15 DELY=-NDY+1,NDY-1
DO 15 DELX=-NDX+1,NDX-1
C
      COVH =COVG (KH, 0)
      COVU =COVG ( IABS (DELX) , IABS (DELY) )
      COVUMH=COVG ( IABS (DELX-KH) , IABS (DELY) )
      COVUPH=COVG ( IABS (DELX+KH) , IABS (DELY) )
C
C      LOI DE GAUSS      Z=U      U N(0,1)
C
      IF (KLOI.EQ.0) THEN
          GGG=0.5*(2*COVU-COVUMH-COVUPH)**2
C
C      LOI GAMMA      Z=U**2/SQRT(2.)      U N(0,1)
C      ==> GAMMA (H) =1-RHO (H) **2
C
      ELSEIF (KLOI.EQ.1) THEN
          GGG= 8*(2*COVU**2+COVUMH**2+COVUPH**2)
&          + 6*(COVUMH**4+COVUPH**4)
&          +16*(COVU**2+COVH**2)*(COVU**2+COVUMH*COVUPH)
&          + 4*(COVUMH**2)*(COVUPH**2)
&          -24*(COVU**2)*(COVUMH**2+COVUPH**2)
&          -32*COVU*COVH*(COVUMH+COVUPH)
          GGG=GGG/4.
C
C      LOI DE BESSEL      Z=U1*U2      U1,U2 N(0,1)
C      ==>      GAMMA (H) =1-RHO (H) **2
C
      ELSEIF (KLOI.EQ.2) THEN
          GGG= 2*COVU**2+COVUMH**2+COVUPH**2
&          +3*COVU**4+COVUMH**4+COVUPH**4
&          -4*COVU**2*(COVUMH**2+COVUPH**2)
&          +2*(COVU**2)*(COVH**2)+(COVUMH**2)*(COVUPH**2)
&          +2*(COVU**2+COVH**2)*COVUMH*COVUPH
&          -4*COVU*COVH*(COVUMH+COVUPH)
C
C      LOI LOGNORMALE      Z=EXP (U) /SQRT (E*(E-1))      U N(0,1)
C      ==>      GAMMA (H) =1-(EXP (RHO (H) ) -1) / (E-1)
C      EN PARTICULIER, SI U AVEC MODELE MIXTE DE PORTEE ALPHA,
C      GAMMA (H) =1-EXP (-H/ALPHA)
C      EXCEPTION : SCHEMA EXPONENTIEL A 1-D ET ALPHA>1 :
C      Z=EXP (U) /E      U N(0,1) AVEC COVARIANCE TRIANGLE
C      DE PORTEE ALPHA
C      ==>      GAMMA (H) =1-EXP (-H/ALPHA)      SUR [0,1]
C
      ELSEIF (KLOI.EQ.3) THEN
          GGG= 0.50*DEXP (2+4*COVU)
&          +0.25*DEXP (2+4*COVUMH) +0.25*DEXP (2+4*COVUPH)
&          -      DEXP (1+COVH+2*COVU+2*COVUMH)
&          -      DEXP (1+COVH+2*COVU+2*COVUPH)
&          +      DEXP (2*COVH+2*COVU+COVUMH+COVUPH)
&          - (DEXP (1.D0) -DEXP (COVH) ) **2
          GGG=DEXP (2.D0) *GGG
          IF (ITYPE.EQ.2) GGG=GGG/DEXP (4.D0)
          IF (ITYPE.EQ.8) GGG=GGG/ (DEXP (1.D0) * (DEXP (1.D0) -1.)) **2
C
      ENDIF
C
      COVQ (DELX, DELY) =GGG
C
15      CONTINUE

```

```

C
C   DOUBLE SOMME DES G (ID-JD;KH) , ID,JD DECRIVANT LE DOMAINE VH
C
      GDD=0.
      DO 22 DELY=-NDY+1,NDY-1
        NY=NDY-IABS (DELY)
        GGG=0.
        DO 21 DELX=-NDX+1,NDX-1
          NX=NDX-IABS (DELX)
          GGG=GGG+NX*COVQ (DELX,DELY)
21      CONTINUE
        GDD=GDD+NY*GGG
22      CONTINUE
        GDD=GDD/ ((NDX*NDY)**2)
C
C   DOUBLE SOMME DES G (IP-JP;KH) , IP,JP DECRIVANT LES POINTS EXP.
C
      GPP=GDD
      IF (NPX0.EQ.NDX0.AND.NPY0.EQ.NDY0) GO TO 40
      GPP=0.
      DO 32 DELY=-NDY+1,NDY-1,IYPAS
        NY=1+(NDY-1)/IYPAS-IABS (DELY)/IYPAS
        GGG=0.
        DO 31 DELX=-NDX+1,NDX-1,IXPAS
          NX=1+(NDX-1)/IXPAS-IABS (DELX)/IXPAS
          GGG=GGG+NX*COVQ (DELX,DELY)
31      CONTINUE
        GPP=GPP+NY*GGG
32      CONTINUE
        GPP=GPP/ ((NPX*NPY)**2)
C
C   DOUBLE SOMME DES G (ID-IP;KH)
C
40      GDP=GDD
      IF (NPX0.EQ.NDX0.AND.NPY0.EQ.NDY0) GO TO 50
      GDP=0.
      DO 42 DELY=-NDY+1,NDY-1
        NY=1+(NDY-1-IABS (DELY))/IYPAS
        GGG=0.
        DO 41 DELX=-NDX+1,NDX-1
          NX=1+(NDX-1-IABS (DELX))/IXPAS
          GGG=GGG+NX*COVQ (DELX,DELY)
41      CONTINUE
        GDP=GDP+NY*GGG
42      CONTINUE
        GDP=GDP/ (NDX*NDY*NPX*NPY)
C
C   CALCUL DU VARIOGRAMME ET DES VARIANCES DE LA VARIABLE
C   NON GAUSSIENNE
C
50      GAM=COVGEN (0.D0, ITYPE, ALPHA) -COVGEN (H, ITYPE, ALPHA)
        GAM2=GAM**2
        VARFLU=GDD
        SIGFLU=DSQRT (VARFLU)
        VAREST=GDD+GPP-2.*GDP
        IF (VAREST.LT.0.) VAREST=0.
        SIGEST=DSQRT (VAREST)
360     WRITE (3,360) H, SIGFLU/GAM, SIGEST/GAM
        FORMAT (1H ,F5.3,2F8.4)
C
90     CONTINUE

```

```

C
C
RETURN
END
DOUBLE PRECISION FUNCTION COVGEN(H, ITYPE, ALPHA)
C
C
COVARIANCE OU -VARIOGRAMME
C
C
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C
GO TO (10,20,30,40,50,60,70,70), ITYPE
C
C
MODELE SPHERIQUE
C
10 IF(H.LT.ALPHA) THEN
    R=H/ALPHA
    COV=1.-1.5*R+0.5*R**3
ELSE
    COV=0.
ENDIF
GO TO 90
C
C
MODELE EXPONENTIEL
C
20 R=H/ALPHA
COV=DEXP(-R)
GO TO 90
C
C
MODELE CUBIQUE
C
30 IF(H.LT.ALPHA) THEN
    R=H/ALPHA
    R2=R**2
    COV=1.-R2*(7.-R*(8.75+R2*(-3.5+0.75*R2)))
ELSE
    COV=0.
ENDIF
GO TO 90
C
C
MODELE GAUSSIEN
C
40 R=H/ALPHA
COV=DEXP(-0.5*R**2)
GO TO 90
C
C
MODELE EN H**ALPHA
C
50 IF(H.EQ.0.) THEN
    COV=0.
ELSE
    COV=-H**ALPHA
ENDIF
GO TO 90
C
C
MODELE TRIANGLE
C
60 IF(H.LT.ALPHA) THEN
    R=H/ALPHA

```

```

        COV=1.-R
    ELSE
        COV=0.
    ENDIF
    GO TO 90
C
C     MODELE MIXTE
C     (MODELE CONCU DE MANIERE QUE SI U(X) EST GAUSSIENNE ET ADMET CE
C     MODELE DE VARIOGRAMME, ALORS EXP(U(X)) EST LOGNORMALE ET A UN
C     VARIOGRAMME TRES PROCHE DU MODELE EXPONENTIEL. LE SCHEMA MIXTE DE
C     PORTEE ALPHA COMPORTE :
C     - 50% DE SCHEMA EXPONENTIEL DE PORTEE 1.6*ALPHA;
C     - 50% DE SCHEMA SPHERIQUE DE PORTEE 2.7*ALPHA.)
C
70  AEXP=1.6*ALPHA
    R=H/AEXP
    CEXP=DEXP(-R)
    ASPH=2.7*ALPHA
    IF(H.LT.ASPH) THEN
        R=H/ASPH
        CSPH=1.-1.5*R+0.5*R**3
    ELSE
        CSPH=0.
    ENDIF
    COV=0.5*(CEXP+CSPH)
    IF(ITYPE.EQ.8) GO TO 80
    GO TO 90
C
C     MODELE LOGNORMAL ASSOCIE AU MODELE MIXTE
C
80  COV=(DEXP(COV)-1.)/(DEXP(1.D0)-1.)
    GO TO 90
C
C
90  COVGEN=COV
C
    RETURN
    END

```