Multivariate Analysis and Spatial/Temporal Scales: Real and Complex Models

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Published in:

Proceedings of XVIIth International Biometric Conference,

8–12 August 1994 at Hamilton, Ontario, Canada,

Volume 1 (Invited Papers), pages 19–33.

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Summary

Comparing different scales in space or time the correlation between regionalized quantities can change substantially. Coregionalization models incorporate a description of the variation and covariation of a set of variables at different characteristic scales either in space or in time. Such models can be used as a device to explore the structure of multivariate spatial or temporal data in the framework of a regionalized multivariate data analysis.

We review the work done using the classical Linear Model of Coregionalization (LMC) which is adequate to model sets of variograms and cross variograms as well as sets of covariance functions with *even* cross covariance functions. We also present a new generalization of the LMC due to Grzebyk (1993), the Bilinear Model of Coregionalization (BMC), which is suitable for modeling a coregionalization in space or along the time axis using cross covariance functions which are not even.

1 Introduction

We do not want to open the Pandora's box of space-time models, i.e. we shall not consider covariance functions (or variograms) which depend on both space and time. The two classes of models, the LMC and the BMC, are suitable to be applied either to multivariate spatial data or to multiple/multivariate time series.

The LMC implies even cross covariance functions. It can thus be formulated in a framework with variograms implying a less restrictive definition of stationarity: only the increments of the random functions are assumed to be jointly stationary. The use of cross variograms (even cross covariance functions) excludes deferred correlations which are however less likely to occur between spatial variables. Thus the LMC underlying a variogram matrix model can be appropriate for spatial multivariate data.

The BMC allows for uneven cross covariance functions. It is interesting for modeling second order stationary multivariate spatial data as well as multiple/multivariate time series with deferred correlations. Deferred correlations can be thought of as effects of one variable on other variables which occur with a certain delay in time (or space). Deferred correlations (like correlations in general) do not follow an equivalence relation and their modeling is thus not trivial.

In Section 2 we define the set of variograms and cross variograms for random functions with jointly stationary increments. We also write down the simplest LMC, the intrinsic correlation model, in which multivariate correlation does not depend on spatial/temporal scale. In Section 3 we expose briefly the steps of structural analysis: the geostatistical way of choosing a nested model and its parameters for fitting a variogram to values computed on data. As an example we discuss a standard model from geochemical exploration. Section 4 generalizes the concept of a nested variogram model to the multivariate case and shows its association with the LMC. In Section 5 various implementations of the LMC for the purpose of regionalized multivariate data analysis are reviewed.

Section 6 is about an alternate generalization of the cross variogram called the "pseudo cross-variogram" (Myers, 1992) and which is not an even function. We explain why we do not use this approach and why we prefer the classical cross covariance functions, which are formally defined in Section 7.

Section 8 presents a model for real covariance function matrices obtained by taking the real part of a complex intrinsic correlation model. Section 9 describes a nested version of this covariance function model and the underlying BMC. Section 10 discusses the BMC from the point of view of structural and regionalized multivariate analysis. Sections 11 to 13 finally give different implementations of the BMC for the cases of deferred correlation, different support and variables being the derivatives of others.

2 The matrix of direct and cross variograms

Let $Z_i(\mathbf{x})$, $i = 1, \ldots, N$ be random functions, $\mathcal{D}$ be a closed portion of space (or an interval of time) and $\mathbf{x}$, $\mathbf{x}+\mathbf{h}$ be two points in $\mathcal{D}$. The set of random functions $\big\{Z_i(\mathbf{x})\big\}$ is said to be *intrinsically stationary of order 2* if the following two assumptions about the increments $Z_i(\mathbf{x}+\mathbf{h}) - Z_i(\mathbf{x})$ are true (Matheron, 1965):

$$\forall \mathbf{x} \in \mathcal{D}, \forall i : \qquad \mathrm{E}\Big[\, Z_i(\mathbf{x}+\mathbf{h}) - Z_i(\mathbf{x}) \Big] = 0 \tag{1}$$

$$\forall \mathbf{x} \in \mathcal{D}, \forall i, j : \qquad \mathrm{cov}\Big(Z_i(\mathbf{x}+\mathbf{h}) - Z_i(\mathbf{x}), Z_j(\mathbf{x}+\mathbf{h}) - Z_j(\mathbf{x}) \Big) = 2\,\gamma_{ij}(\mathbf{h}) \tag{2}$$

The translation invariant function

$$\gamma_{ij}(\mathbf{h}) = \frac{1}{2}\,\mathrm{E}\Big[\Big(Z_i(\mathbf{x}+\mathbf{h}) - Z_i(\mathbf{x}) \Big) \cdot \Big(Z_j(\mathbf{x}+\mathbf{h}) - Z_j(\mathbf{x}) \Big) \Big] \tag{3}$$

is called the *direct variogram* (or *variogram*) for $i = j$ and the *cross variogram* for $i \neq j$. The direct and the cross variograms are even functions.

We can define a matrix of variograms $\boldsymbol{\Gamma}(\mathbf{h}) = \left[\gamma_{ij}(\mathbf{h})\right]$ with the direct variograms on the diagonal and the cross variograms off-diagonal.

The simplest coregionalization model is the *intrinsic correlation* model

$$\boldsymbol{\Gamma}(\mathbf{h}) \;=\; \mathbf{C}\,\gamma(\mathbf{h}) = [c_{ij}]\,\gamma(\mathbf{h}) \tag{4}$$

in which a positive semi-definite matrix of coefficients c_{ij} multiplies a variogram $\gamma(\mathbf{h})$. In this model the correlation r_{ij} between variables does not depend on spatial scale (hence the term 'intrinsic')

$$\frac{\gamma_{ij}(\mathbf{h})}{\sqrt{\gamma_{ii}(\mathbf{h})\,\gamma_{jj}(\mathbf{h})}} \;=\; \frac{c_{ij}}{\sqrt{c_{ii}\,c_{jj}}} = r_{ij} \qquad \text{for any } \mathbf{h} \tag{5}$$

The linear model of coregionalization associated with intrinsic correlation is a decomposition of the form

$$Z_i(\mathbf{x}) \;=\; \sum_{p=1}^{N} \alpha_p^i\, Y_p(\mathbf{x}) \tag{6}$$

where the intrinsically stationary random functions $Y_p(\mathbf{x})$ have the same variogram $\gamma(\mathbf{h})$, where different $Y_p(\mathbf{x})$ are pairwise orthogonal and where $c_{ij} = \sum_{p=1}^{N} \alpha_p^i\, \alpha_p^j$. In a Principal Component Analysis of $\mathbf{C}$ the loadings α_p^i are computed as $\alpha_p^i = \sqrt{\lambda_p}\, q_p^i$ where λ_p is an eigenvalue and q_p^i is an element of an eigenvector $\mathbf{q}_p$ of $\mathbf{C}$.

3 Geostatistical structural analysis

The interpretation of sample values of the variogram of a variable $Z(\mathbf{x})$ is called a *structural analysis*. It consists in choosing and fitting a variogram model $\gamma(\mathbf{h})$ to the experimental variogram values. The interpretation of the behavior at the origin of the variogram (discontinuous, continuous or differentiable) as well as the behavior at large distances (bounded or not) are fundamental steps of the geostatistical approach (Matheron, 1970; Journel and Huijbregts, 1978). They determine the generic model (equivalence class of random functions), its type and its parameters (Matheron, 1989).

Geostatistical structural analysis leads usually to the choice of more than one elementary variogram model: we have a *nested variogram* model consisting of several elementary variograms $\gamma_u(\mathbf{h})$ (with $u = 0, 1, \ldots, S$) multiplied by coefficients c_u

$$\gamma(\mathbf{h}) \;=\; \sum_{u=0}^{S} c_u\, \gamma_u(\mathbf{h}) \tag{7}$$

A typical nested model in geochemical exploration may consist of three structures describing three characteristic scales of the spatial (or temporal) variation

$$\gamma(\mathbf{h}) \;=\; c_0\,\gamma_0(\mathbf{h}) + c_1\,\gamma_1(\mathbf{h}) + c_2\,\gamma_2(\mathbf{h}) \tag{8}$$

with, for example:

- a first structure modeling a discontinuity at the origin of $\gamma(\mathbf{h})$ (the so called *nugget effect*). The model for this discontinuity is a constant c_0 times an indicator function $\gamma_0(\mathbf{h})$ (nil for $|\mathbf{h}| = 0$ and one for $|\mathbf{h}| > 0$). This structure catches the micro-variability at scales lower than the sampling mesh size.
- a second structure describing short range variation. Typically such a function steadily increases from the origin and rapidly reaches a *sill* c_1 at a *range* d_1. The value of this second structure then equals c_1 for all distances $|\mathbf{h}| > d_1$. This structure reflects the small-scale variations associated with spatial objects of a diameter lower or equal to d_1.
- a third structure of the same type as the previous with a sill c_2 and range d_2 much larger than d_1 to account for long range (i.e. large-scale) variation.

The concept of a nested variogram is since long time in use (Serra, 1967) and is analogue to the spectral decomposition of geophysics (Spector and Grant, 1970). The basic idea is that the variation due to uncorrelated processes $Y_u(\mathbf{x})$ acting at different scales of a spatial (or temporal) phenomenon add up in a simple manner to form a linear model of regionalization

$$Z(\mathbf{x}) \;=\; \sum_{u=0}^{S} \alpha_u\, Y_u(\mathbf{x}) \tag{9}$$

where each $Y_u(\mathbf{x})$ has a different variogram $\gamma_u(\mathbf{h})$ and the increments of different $Y_u(\mathbf{x})$ are pairwise orthogonal. The coefficients c_u of the nested variogram model (7) are the squares of the coefficients α_u.

4 Multivariate nested variogram model

When dealing with several variables $Z_i(\mathbf{x})$ stemming from the same region we can consider a structural analysis using uncorrelated factors $Y_u^p(\mathbf{x})$ that build up the variables at different scales of index u. This leads to a combination of models (6) and (9) into a single model, the classical *linear model of coregionalization* (LMC) as in Marbeau (1976), Journel and Huijbregts (1978)

$$Z_i(\mathbf{x}) \;=\; \sum_{u=0}^{S}\sum_{p=1}^{N} \alpha_{pu}^{i}\, Y_u^p(\mathbf{x}) \tag{10}$$

The variogram model that goes with the LMC is the multivariate nested variogram

$$\mathbf{\Gamma}(\mathbf{h}) \;=\; \sum_{u=0}^{S} \mathbf{C}_u\,\gamma_u(\mathbf{h}) = \sum_{u=0}^{S} [c_{ij}^u]\,\gamma_u(\mathbf{h}) \tag{11}$$

with positive semi-definite matrices $\mathbf{C}_u$ of coefficients $c_{ij}^u = \sum_{p=1}^{N} \alpha_{pu}^i\, \alpha_{pu}^j$. The flexibility of this model should not be underestimated. If for example a structure $\gamma_u(\mathbf{h})$ is not present on a particular variogram or cross variogram $\gamma_{ij}(\mathbf{h})$ this simply implies a corresponding coefficient c_{ij}^u equal to zero. Goulard (1988, 1989), Goulard and Voltz (1992) have proposed several fitting procedures.

5 Regionalized multivariate analysis

In a short note Matheron (1982) discussed the possibility of using the linear model of coregionalization as a basis for performing a truly regionalized multivariate data analysis. In particular the cokriging equations for estimating the regionalized factors $Y_u^p(\mathbf{x})$ were presented. This proposal led to several dissertations on the subject (Wackernagel, 1985; Goulard, 1988; Goovaerts, 1992a) and to many publications in the fields of geochemical prospection (Sandjivy, 1984; Wackernagel, 1988; Bourgault and Marcotte, 1991; Wackernagel and Sanguinetti, 1993), in soil science (Wackernagel et al. 1988; Goovaerts, 1992b; Goulard and Voltz, 1993; Raspa et al., 1993), in hydrogeology (Rouhani and Wackernagel, 1990; Goovaerts et al. 1993), in mining (Sousa, 1989) and in image processing (Daly et al., 1989).

Various methods of data analysis can be adapted for decomposing the coregionalization matrices $\mathbf{C}_u$ (Wackernagel et al., 1989). The methods generally used are either Principal Component Analysis or Factor Analysis (with varimax rotation), but methods for analysing two groups of variables like Canonical Analysis or Redundancy Analysis (Goovaerts, 1994; Lindner and Wackernagel, 1993) were also applied. The approach has been combined with Cluster Analysis to solve classification problems (Sousa, 1989; Raspa et al., 1993).

A fundamental question when analysing multivariate spatial data is to check whether the variables are intrinsically correlated (Wackernagel, 1994). If the answer is positive, the coregionalization model (10) reduces to the model (6). As a consequence the factors $Y_p(\mathbf{x})$ can be determined at sampling locations by classical non-regionalized multivariate methods and subsequently kriged instead of cokriged at unsampled locations of the region of interest.

6 About the pseudo cross-variogram

The cross variogram is an even function. It is thus inapropriate when there is some shift in the correlation between two variables: like in time series when the variation of one variable has a delayed effect on another variable. An alternate generalization of the variogram, the pseudo cross-variogram $\pi_{ij}(\mathbf{h})$, has been proposed by Myers (1991) and Cressie (1991) by considering the variance of the cross increments instead of the covariance of the direct increments as in Equation (2). This function has the advantage not to be even. Assuming for the expectation of the cross increments

$$\forall \mathbf{x} \in \mathcal{D}, \forall i, j: \qquad \mathrm{E}\Big[Z_i(\mathbf{x}+\mathbf{h}) - Z_j(\mathbf{x}) \Big] = 0 \tag{12}$$

the pseudo cross-variogram comes as

$$\pi_{ij}(\mathbf{h}) = \frac{1}{2}\,\mathrm{E}\Big[\Big(Z_i(\mathbf{x}+\mathbf{h}) - Z_j(\mathbf{x}) \Big)^2 \Big] \tag{13}$$

The assumption (12) of stationary cross increments is unrealistic: it usually does not make sense to take the difference between two variables measured in different physical units. Papritz et al. (1993), Papritz and Flühler (1994) have experienced limitations in the usefulness of the pseudo cross-variogram and they argue that it applies only to second-order stationary functions.

Another drawback of the pseudo cross-variogram function is that it is not adequate for modeling negatively correlated variables.

For these reasons we shall not consider further this approach and switch to the classical cross covariance function (Cramer, 1940).

7 The matrix of direct and cross covariance functions

The random functions $Z_i(\mathbf{x}), i = 1, \ldots, N$ are said to be *jointly stationary of order 2* if the following two assumptions are true:

$$\forall \mathbf{x} \in \mathcal{D}, \forall i: \qquad \mathrm{E}\Big[Z_i(\mathbf{x}) \Big] = m_i \tag{14}$$

$$\forall \mathbf{x} \in \mathcal{D}, \forall i, j: \qquad \mathrm{cov}\Big(Z_i(\mathbf{x}+\mathbf{h}), Z_j(\mathbf{x}) \Big) = C_{ij}(\mathbf{h}) \tag{15}$$

The translation invariant function

$$C_{ij}(\mathbf{h}) = \mathrm{E}\Big[\Big(Z_i(\mathbf{x}+\mathbf{h}) - m_i \Big) \cdot \Big(Z_j(\mathbf{x}) - m_j \Big) \Big] \tag{16}$$

is called the *centered direct covariance function* (or *covariance function*) for $i = j$ and the *cross covariance function* for $i \neq j$.

We can define a matrix of covariance functions $\mathbf{C}(\mathbf{h}) = \Big[C_{ij}(\mathbf{h}) \Big]$ with the direct covariance functions on the diagonal and the cross covariance functions off-diagonal.

The direct covariance functions $C_{ii}(\mathbf{h})$ are even, but, unlike the cross variograms, the cross covariance functions are not even in general. For this reason, the intrinsic correlation (4) and (6) model and the classical LMC (10) and (11) are in general not appropriate to model multivariate data sets using covariance functions since they lead to even cross covariance functions.

8 A model for the covariance function matrix

In order to introduce a model of covariance function matrices, it is possible to make use of *complex covariance functions*. Let $c(\mathbf{h})$ be a complex covariance function. A simple model of complex covariance function matrix is

$$\mathbf{C}(\mathbf{h}) \quad = \quad \mathbf{C}\, c(\mathbf{h}) = [c_{ij}]\, c(\mathbf{h}) \tag{17}$$

in which $\mathbf{C}$ is a hermitian positive semi-definite matrix of coefficients c_{ij} (in particular, $c_{ji} = \overline{c_{ij}}$).

Then, the real part of this complex covariance function matrix is a *real* covariance function matrix which can be written (Grzebyk, 1993) :

$$\mathbf{C}_{re}(\mathbf{h}) \quad = \quad \mathbf{A}\, f(\mathbf{h}) - \mathbf{B}\, g(\mathbf{h}) = [a_{ij}]\, f(\mathbf{h}) - [b_{ij}]\, g(\mathbf{h}) \tag{18}$$

with $\mathbf{C} = \mathbf{A} + \mathrm{i}\mathbf{B}$, $\forall i, j\ c_{ij} = a_{ij} + \mathrm{i} b_{ij}$ and $c(\mathbf{h}) = f(\mathbf{h}) + \mathrm{i} g(\mathbf{h})$.

The direct covariance functions are $C_{ii}(\mathbf{h}) = a_{ii}\, f(\mathbf{h})$. As the imaginary part $g(\mathbf{h})$ of the complex covariance function $c(\mathbf{h})$ is odd, the cross covariance functions have an even and an odd part: when $i \neq j$, $C_{ij}(\mathbf{h}) = a_{ij}\, f(\mathbf{h}) - b_{ij}\, g(\mathbf{h})$.

Regarding the random functions, this covariance function matrix corresponds to the following decomposition (Grzebyk, 1993). Let $\left\{X_p(\mathbf{x})\right\}$ and $\left\{Y_p(\mathbf{x})\right\}$ be two sets of N random functions, stationary of order 2, such that they verify the conditions:

(A) the factors $X_p(\mathbf{x})$ or $Y_p(\mathbf{x})$ have the same covariance function $f(\mathbf{h})$,

(B) the factors are pairwise orthogonal, *except for the pairs* $(X_p(\mathbf{x}), Y_p(\mathbf{x}))$, for which the cross covariance function is $g(\mathbf{h})$.

Then, the random functions

$$Z_i(\mathbf{x}) \quad = \quad \sum_{p=1}^{N} \Big(\alpha_p^i\, X_p(\mathbf{x}) + \beta_p^i\, Y_p(\mathbf{x}) \Big) \quad \text{for } i = 1, ..., N \tag{19}$$

in which α_p^i and β_p^i are real constants, have the covariance function matrix (18) with

$$c_{ij} \quad = \quad \sum_{p=1}^{N} (\alpha_p^i + \mathrm{i}\beta_p^i)\overline{(\alpha_p^j + \mathrm{i}\beta_p^j)} \tag{20}$$

$$\text{and} \quad a_{ij} \quad = \quad \sum_{p=1}^{N} \alpha_p^i \alpha_p^j + \beta_p^i \beta_p^j \qquad b_{ij} \quad = \quad \sum_{p=1}^{N} \alpha_p^j \beta_p^i - \beta_p^j \alpha_p^i \tag{21}$$

The covariance between $Z_i(\mathbf{x})$ and the factor $X_p(\mathbf{x})$ is $\alpha_p^i f(0)$, the one between $Z_i(\mathbf{x})$ and $Y_p(\mathbf{x})$ is $\beta_p^i f(0)$. They can be computed as $\alpha_p^i + \mathrm{i}\beta_p^i = \sqrt{\lambda_p}(r_p^i + \mathrm{i} s_p^i)$, where λ_p is an eigenvalue and $r_p^i + \mathrm{i} s_p^i$ is an element of the eigenvector of $\mathbf{C}$ associated to λ_p.

Actually, this model is based on the sum of two correlated LMCs as written in (6), whose factors have the same covariance function $f(\mathbf{h})$, and which are correlated through each pair of factors $(X_p(\mathbf{x}), Y_p(\mathbf{x}))$. Furthermore, the correlation between these two factors is very special: their cross covariance function $g(\mathbf{h})$ is *odd*. The crucial point of this model is that these two covariance functions (direct and cross) have only to verify the property that $c(\mathbf{h}) = f(\mathbf{h}) + \mathrm{i}g(\mathbf{h})$ is a *complex covariance function*. Several classes of parametric complex covariance functions are proposed by Lajaunie and Bejaoui (1991) and Grzebyk (1993).

These conditions on the correlations between each pair of factors $(X_p(\mathbf{x}), Y_p(\mathbf{x}))$ might be considered too strong; other models could be developped, using also two LMCs, but with less restricting conditions on this correlation. For example, the cross covariance function could be assumed not to be odd. Furthermore, the covariance function of each set of factors $X_p(\mathbf{x})$ and $Y_p(\mathbf{x})$ could be different functions. These conditions generate other models for covariance function matrices than (18), but also imply additional practical and theorical difficulties.

9 The Bilinear Model of Coregionalization

The concept of a nested covariance function for several variables leads to the formulation of the Bilinear Model of Coregionalization (Grzebyk, 1993). It uses several sets of factors $\left\{X_u^p(\mathbf{x})\right\}$ and $\left\{Y_u^p(\mathbf{x})\right\}$, corresponding to different scales of index u. For each scale of index u, the factors $\left\{X_u^p(\mathbf{x})\right\}$ and $\left\{Y_u^p(\mathbf{x})\right\}$ fullfil the conditions (A) and (B), with $f_u(\mathbf{h})$ for the direct covariance function and $g_u(\mathbf{h})$ for the cross covariance function.

The Bilinear Model of Coregionalization is built up as:

$$Z_i(\mathbf{x}) \quad = \quad \sum_{u=0}^{S} \sum_{p=1}^{N} \left(\alpha_{pu}^i \, X_u^p(\mathbf{x}) + \beta_{pu}^i \, Y_u^p(\mathbf{x}) \right) \tag{22}$$

whose covariance function matrix is:

$$\mathbf{C}(\mathbf{h}) \quad = \quad \sum_{u=0}^{S} \left(\mathbf{A}_u \, f_u(\mathbf{h}) - \mathbf{B}_u g_u(\mathbf{h}) \right) = \sum_{u=0}^{S} \left([a_{ij}^u] \, f_u(\mathbf{h}) - [b_{ij}^u] \, g_u(\mathbf{h}) \right) \tag{23}$$

with positive semi-definite matrices $\mathbf{C}_u = \mathbf{A}_u + \mathrm{i}\mathbf{B}_u$ of coefficients $c_{ij}^u = a_{ij}^u + \mathrm{i}b_{ij}^u$ connected to the coefficients α_{pu}^i and β_{pu}^i through the relations (20) and (21).

Several fitting procedures are proposed in Grzebyk (1993).

10 Decomposition into factors and structural analysis

The factors of the two sets of random functions $\left\{X_u^p(\mathbf{x})\right\}$ and $\left\{Y_u^p(\mathbf{x})\right\}$ are pairwise orthogonal, except for each pair $(X_u^p(\mathbf{x}), Y_u^p(\mathbf{x}))$, for which the cross covariance function is an odd function $g_u(\mathbf{h})$. Furthermore, as with the LMC, they can be gathered according to their direct covariance function $f_u(\mathbf{h})$ so that Z_i can be rewritten:

$$Z_i(\mathbf{x}) \;=\; \sum_{u=0}^{S} Z_i^u(\mathbf{x}) \quad \text{with} \quad Z_i^u(\mathbf{x}) \;=\; \sum_{p=1}^{N} \left(\alpha_{pu}^i \, X_u^p(\mathbf{x}) + \beta_{pu}^i \, Y_u^p(\mathbf{x}) \right) \tag{24}$$

For each real variable $Z_i(\mathbf{x})$, the components $Z_i^u(\mathbf{x})$ act independently at different scales of the spatial or temporal phenomenon, with cross covariance functions proportional to $f_u(\mathbf{h})$ and $g_u(\mathbf{h})$.

Again, the BMC can be used to perform a regionalized data analysis, by estimating (cokriging) the regionalized components $Z_i^u(\mathbf{x})$ as well as the factors $X_u^p(\mathbf{x})$ and $Y_u^p(\mathbf{x})$.

With its decomposition into independent components, the BMC can be infered on the basis of structural analysis, by choosing the elementary covariance functions $c_u(\mathbf{h}) = f_u(\mathbf{h}) + \mathrm{i} g_u(\mathbf{h})$. In fact, because of the splitting into two terms (the even and the odd ones) of the covariance function matrix, two structural analyses have to be performed. The structural analysis of the even part is similar to that described in section 3 and leads to the determination of the real parts $f_u(\mathbf{h})$ of the complex covariance functions, describing the characteristic scales of the spatial variation. The structural analysis of the odd part only acts on the cross covariance functions. However, its physical interpretation (in terms of structure or characteristic scale) is difficult.

In the general case, the correlation between two variables can be of a much different nature than that of the BMC. Three examples are given below: the deferred correlation, the correlation produced by variables whose support are different and the correlation of variables and their derivatives.

11 Deferred correlations

The correlation is said to be *deferred* when the extreme value of the cross correlation between two variables $Z_i(\mathbf{x})$ and $Z_j(\mathbf{x})$ does not occur at the origin, but for some $\mathbf{h}_{ij} \neq 0$.

Consider the following simple model (Journel and Huijbregts, 1978). Let $Y_p(\mathbf{x})$ be N stationary random functions of order 2 having the same covariance function $f(\mathbf{h})$, pairwise orthogonal; let $(\mathbf{h}_i)$ be N vectors of the space, and (α_p^i) real coefficients. Then the random functions $Z_i(\mathbf{x}) = \sum_{p=1}^{N} \alpha_p^i Z_p(\mathbf{x} + \mathbf{h}_i)$ have the covariance function matrix

$$\mathbf{C}(\mathbf{h}) = \Big[C_{ij}(\mathbf{h}) \Big] \qquad \text{with} \qquad C_{ij}(\mathbf{h}) = c_{ij} f(\mathbf{h} + \mathbf{h}_i - \mathbf{h}_j) \tag{25}$$

in which the coefficients $c_{ij} = \sum_{p=1}^{N} \alpha_p^i \alpha_p^j$ form a real positive semi-definite matrix $\mathbf{C}$, such as in (4). The extremum of correlation between $Z_i(\mathbf{x})$ and $Z_j(\mathbf{x})$ occurs at $\mathbf{h} = \mathbf{h}_i - \mathbf{h}_j$. The covariance between $Z_i(\mathbf{x})$ and $Y_p(\mathbf{x})$ is no more $\alpha_p^i f(0)$ but $\alpha_p^i f(\mathbf{h}_i)$.

In fact this is a shifted intrinsic correlation model since the variables $Z_i(\mathbf{x}-\mathbf{h}_i)$ are intrinsically correlated, with the real covariance function matrix $\mathbf{C}(\mathbf{h}) = \mathbf{C}f(\mathbf{h})$. Note that in order to be interpreted as a shifted intrinsic correlation model, the shifting $\mathbf{h}_{ij}$ of the deferred correlations have to follow the conditions of compatibility (some $\mathbf{h}_i$ might be nil)

$$\mathbf{h}_{ij} = \mathbf{h}_i - \mathbf{h}_j \quad \forall i, j \tag{26}$$

In this case the shifted covariance function matrix (25) can be used, or more generally, a nested model of such shifted covariance function matrices.

In the contrary (when $\mathbf{h}_{ij}$ cannot be written $\mathbf{h}_i - \mathbf{h}_j$ for all i and j), the deferred correlations cannot be interpreted as resulting from a spatial (or temporal) shifting of all variables. For instance, with three variables, there might be a deferred correlation between $Z_1(\mathbf{x})$ and $Z_2(\mathbf{x})$, but no deferred correlation between $Z_1(\mathbf{x})$ and $Z_3(\mathbf{x})$ as well as between $Z_2(\mathbf{x})$ and $Z_3(\mathbf{x})$. Then the covariance function matrix cannot be modeled by the shifted covariance function matrix (25). Sometimes, the plain BMC can be used or else a more specific model has to be developped.

12 Variables with different supports

Up to now, the variables were assumed to be punctual. Otherwise the way they are collected (variables integrated on different lengths, surfaces, volumes, intervals, or using a device which convolutes them) does matter. This can have a great impact on the covariance function matrix, especially when the size of these supports is very different. The modelling has to take these different supports into account. The LMC (for the variogram) and the BMC (for the covariance) have to be slightly modified. To be more precise, only the underlying punctual variables can be assumed to follow the LMC or the BMC.

Let $Z_i(\mathbf{x}), i = 1, ..., N$ be the underlying punctual variables whose matrix of covariance functions is $\mathbf{C}(\mathbf{h}) = \left[C_{ij}(\mathbf{h})\right]$. The measured variables are $\tilde{Z}_i(\mathbf{x}) = (Z_i * p_i)(\mathbf{x})$, where $p_i(\mathbf{x})$ is the function which characterizes the support of the variable $Z_i(\mathbf{x})$. Then, the matrix of covariance functions is

$$\tilde{\mathbf{C}}(\mathbf{h}) \quad = \quad \left[(C_{ij} * p_i * \check{p}_j)(\mathbf{h})\right] \tag{27}$$

If the set of punctual variables $\{Z_i(\mathbf{x})\}$ is modeled using the BMC, as in (22) and (23), it corresponds to the decomposition of the measured variables:

$$\tilde{Z}_i(\mathbf{x}) \quad = \quad \sum_{u=0}^{S} \sum_{p=1}^{N} \left(\alpha_{pu}^i \left(p_i * X_u^p(\mathbf{x})\right) + \beta_{pu}^i \left(p_i * Y_u^p(\mathbf{x})\right) \right) \tag{28}$$

and the matrix of covariance functions:

$$\tilde{C}(\mathbf{h}) \quad = \quad [\tilde{C}_{ij}(\mathbf{h})] \tag{29}$$

with

$$\tilde{C}_{ij}(\mathbf{h}) \;=\; \sum_{u=0}^{S} a_{ij}^{u}\,(p_i * \check{p}_j * f_u)(\mathbf{h}) + b_{ij}^{u}\,(p_i * \check{p}_j * g_u)(\mathbf{h}) \tag{30}$$

Again, the matrices $\mathbf{C}_u$ of coefficients $c_{ij}^u = a_{ij}^u + \mathrm{i} b_{ij}^u$ given by (20) is hermitian positive semi-definite. Note that the covariance functions (direct or cross) are no more linear combinations of the same functions.

The functions $p_i(\mathrm{x})$ characterizing the supports have to be known to perform this adaptation. Provided this is true, it is then possible to study the spatial or temporal variations of the ponctual variables, eliminating the effects of the support of the measures.

13 Variables and derivatives

When physical laws (implying formal equations) link the different variables of a coregionalization, crucial benefits can be gained when taking them into account. Examples are described in Chauvet et al. (1976) who use wind data to estimate the geopotential, Dong (1990) who treats different problems of flow in hydrogeology and Renard and Ruffo (1993) who estimate a topographic surface using its depth and its gradient.

As an illustration, consider the simple example of a variable defined along a line (the time axis for instance) and its derivative. Let $Z_i(\mathbf{x})$, $i = 1, \ldots, N$ be random functions jointly stationary of order 2. Assume that $Z_1(\mathbf{x})$ is mean square differentiable; the random functions $Z_i(\mathbf{x}), i = 1, \ldots, N, Z_1'(\mathbf{x})$ are jointly stationary of order 2. If $C_{ij}(\mathbf{h})$ is the covariance functions between $Z_i(\mathbf{x})$ and $Z_j(\mathbf{x})$, the covariance functions of $Z_1'(\mathbf{x})$ verify:

$$\mathrm{cov}\Big(Z_1'(\mathbf{x}+\mathbf{h}), Z_i(\mathbf{x})\Big) \;=\; C_{ij}'(\mathbf{h}), \text{ for } i = 1, ..., N \tag{31}$$

$$\mathrm{cov}\Big(Z_1'(\mathbf{x}+\mathbf{h}), Z_1'(\mathbf{x})\Big) \;=\; -C_{11}''(\mathbf{h}) \tag{32}$$

It is still possible to use the BMC to model this coregionalization in a way which takes into account the link between $Z_1(\mathbf{x})$ and its derivative $Z_1'(\mathbf{x})$. Whereas there are $N+1$ variables, each regionalized component needs only N pairs of factors $(X_u^p(\mathbf{x}), Y_u^p(\mathbf{x}))$; if

$$Z_i(\mathbf{x}) \;=\; \sum_{u=0}^{S}\sum_{p=1}^{N}\Big(\alpha_{pu}^{i}\,X_u^p(\mathbf{x}) + \beta_{pu}^{i}\,Y_u^p(\mathbf{x})\Big) \tag{33}$$

then,

$$Z_1'(\mathbf{x}) \;=\; \sum_{u=0}^{S}\sum_{p=1}^{N}\Big(\alpha_{pu}^{1}\,X_u^{p\prime}(\mathbf{x}) + \beta_{pu}^{1}\,Y_u^{p\prime}(\mathbf{x})\Big) \tag{34}$$

and the covariance functions for $i, j = 1, ..., N$ are

$$C_{ij}(\mathbf{h}) \;=\; \sum_{u=0}^{S}\Big([a_{ij}^u]\,f_u(\mathbf{h}) - [b_{ij}^u]\,g_u(\mathbf{h})\Big) \tag{35}$$

whereas

$$\operatorname{cov}\Big(Z_1'(\mathbf{x}+\mathbf{h}), Z_1'(\mathbf{x})\Big) = -\sum_{u=0}^{S}[a_{11}^u]\, f_u''(\mathbf{h}) \tag{36}$$

$$\operatorname{cov}\Big(Z_1'(\mathbf{x}+\mathbf{h}), Z_i(\mathbf{x})\Big) = \sum_{u=0}^{S}\Big([a_{1j}^u]\, f_u'(\mathbf{h}) - [b_{1j}^u]\, g_u'(\mathbf{h})\Big) \tag{37}$$

14 Conclusion

The structural analysis determines different characteristic scales of the spatial or temporal variation. They can be used through the LMC (with variograms) or the BMC (with covariance functions) to perform regionalized data analysis. These two models are very attractive because they are simple to implement. Whereas the LMC is already widely in use, the BMC must still find its way to applications. Its strong point is the possibility to take into account asymmetric spatial or temporal relations between the variables (through the cross covariance functions). However, the physical meaning of the asymmetry is not yet fully understood. The simplest case of asymmetry is shifted intrinsic correlation for which formulations of the LMC and the BMC exist.

The adaptation of these models to variables measured on different supports as well as the example of the correlation between a variable and its derivatives are illustrations of the fact that the spatial relations between variables may be more complex than those allowed by a plain LMC or BMC. Conversely, when physical relations between variables are known, it is still possible to integrate them into these linear models.

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