

# The Linear Coregionalization Model and the Product–Sum Space–Time Variogram<sup>1</sup>

S. De Iaco,<sup>2</sup> D. E. Myers,<sup>3</sup> and D. Posa<sup>2,4</sup>

---

*The product covariance model, the product–sum covariance model, and the integrated product and integrated product–sum models have the advantage of being easily fitted by the use of “marginal” variograms. These models and the use of the marginals are described in a series of papers by De Iaco, Myers, and Posa. Such models allow not only estimating values at nondata locations but also prediction in future times, hence, they are useful for analyzing air pollution data, meteorological data, or ground water data. These three kinds of data are nearly always multivariate and because the processes determining the deposition or dynamics will affect all variates, a multivariate approach is desirable. It is shown that the use of marginal variograms for space–time modeling can be extended to the multivariate case and in particular to the use of the Linear Coregionalization Model (LCM) for cokriging in space–time. An application to an environmental data set is given.*

---

**KEY WORDS:** space–time, coregionalization, marginal variograms, product–sum models, integrated models.

## INTRODUCTION

Modeling of spatiotemporal distributions resulting from dynamic processes evolving in both space and time is important in different scientific and engineering fields, such as meteorology, environmental sciences, and hydrology.

Three conceptual viewpoints were identified in Kyriakidis and Journel (1999): (1) approaches involving a single random function model integrating both space and time components (Bilonick, 1985; Christakos, 1992); (2) approaches involving vectors of space random functions (Goovaerts and Sonnet, 1993); (3) approaches involving vectors of time series (Rouhani and Wackernagel, 1990).

---

<sup>1</sup>Received 10 October 2001; accepted 10 October 2002.

<sup>2</sup>Dipartimento di Scienze Economiche e Matematico-Statistiche, Via per Monteroni, Ecotekne, 73100 Lecce, Italy; e-mail: sdeiaco@tiscalinet.it; e-mail: posa@economia.unile.it

<sup>3</sup>Department of Mathematics, University of Arizona, Tucson, Arizona 85721; e-mail: myers@math.arizona.edu

<sup>4</sup>IRMA-CNR, via Amendola 122/I, 70126 Bari, Italy; e-mail: irmadp08@area.ba.cnr.it

However, none of these three incorporates multivariate spatiotemporal distributions. For example, several variables could be measured at given spatial locations and for different times, resulting in multivariate space–time information. Although many authors have used the Linear Coregionalization Model (LCM) for multivariate geostatistical analysis in a spatial context (Goovaerts, 1993), this model has not been used for spatial–temporal processes.

The aim of this paper is to show how marginal variograms for space–time modeling can be extended to the multivariate case. In particular the LCM is extended to space–time applications, where the spatial–temporal basic variograms are modeled as product–sums (De Iaco, Myers, and Posa, 2001a). In this case, each of the variograms in the LCM is written in terms of the space and time marginals and the marginals for the LCM can be easily obtained. However, more general space–time models with the LCM, such as the integrated product and integrated product–sum models (De Iaco, Myers, and Posa, 2002) can be used.

To illustrate the technique, the LCM using a product–sum space–time variogram model has been applied to an environmental data set, involving hourly averages for CO and NO<sub>2</sub>, measured in Milan district during February 1999. Practical aspects related to determining its parameters are also discussed.

### SPACE–TIME LCM

Let

$$\mathbf{Z}(\mathbf{s}, t) = [Z_1(\mathbf{s}, t), \dots, Z_m(\mathbf{s}, t)]^T$$

be a vector valued second-order stationary random function defined on  $R^n \times T$ .

Let

$$\mathbf{Y}(\mathbf{s}, t) = [Y_1(\mathbf{s}, t), \dots, Y_P(\mathbf{s}, t)]^T$$

be a vector of uncorrelated second order stationary random functions and  $\mathbf{D}$  a  $m \times P$  matrix such that

$$\mathbf{Z}(\mathbf{s}, t) = \mathbf{D}\mathbf{Y}(\mathbf{s}, t).$$

Let

$$g_{kl}(\mathbf{h}_s, h_t) = 0.5 \text{Cov}(Z_k(\mathbf{s} + \mathbf{h}_s, t + h_t) - Z_k(\mathbf{s}, t), Z_l(\mathbf{s} + \mathbf{h}_s, t + h_t) - Z_l(\mathbf{s}, t))$$

i.e., the auto and cross-variograms of the components of  $\mathbf{Z}$ , and  $\mathbf{G}(\mathbf{h}_s, h_t)$  the  $m \times m$  matrix whose entries are  $g_{kl}(\mathbf{h}_s, h_t)$ ,  $k, l = 1, \dots, m$ . Let  $\mathbf{g}_j(\mathbf{h}_s, h_t)$ ,

$j = 1, \dots, P$ , be the variograms of the  $Y_j(\mathbf{s}, t)$ ,  $j = 1, \dots, P$ . In the literature, the structures  $\gamma_j(\mathbf{h}_s, h_t)$ ,  $j = 1, \dots, P$ , are known to be the variogram models related to the uncorrelated random functions which define  $Z$  and they do not necessarily have unit sill. As shown in Journel and Huijbregts (1981), the matrix variogram  $\mathbf{G}(\mathbf{h}_s, h_t)$  for  $\mathbf{Z}(\mathbf{s}, t)$  can be written as an LCM:

$$\mathbf{G}(\mathbf{h}_s, h_t) = \sum_{j=1}^P \gamma_j(\mathbf{h}_s, h_t) \mathbf{B}_j \tag{1}$$

where the  $\mathbf{B}_j$ 's are positive definite  $m \times m$  matrices obtained as products of columns of  $\mathbf{D}$  with the transposes of columns. If each basic variogram  $\gamma_j(\mathbf{h}_s, h_t)$  is modeled as a product–sum (De Cesare, Myers, and Posa, 2001a,b, 2002; De Iaco, Myers, and Posa, 2001a,b)

$$\gamma_j(\mathbf{h}_s, h_t) = \gamma_j(\mathbf{h}_s, 0) + \gamma_j(\mathbf{0}, h_t) - K_j \gamma_j(\mathbf{h}_s, 0) \gamma_j(\mathbf{0}, h_t) \tag{2}$$

then each of the variograms  $g_{kl}(\mathbf{h}_s, h_t)$  in the LCM are linear combinations of the space and time marginals. Note that  $\gamma_j(\mathbf{h}_s, 0)$  and  $\gamma_j(\mathbf{0}, h_t)$  are valid spatial and temporal variograms and from (2) the parameter  $K_j$  is given by

$$K_j = \frac{(\text{sill } \gamma_j(\mathbf{h}_s, 0) + \text{sill } \gamma_j(\mathbf{0}, h_t) - \text{sill } \gamma_j(\mathbf{h}_s, h_t))}{(\text{sill } \gamma_j(\mathbf{h}_s, 0) \text{sill } \gamma_j(\mathbf{0}, h_t))}, \quad j = 1, \dots, P. \tag{3}$$

More generally a necessary and sufficient condition for the admissibility of  $\gamma_j(\mathbf{h}_s, h_t)$  is (De Iaco, Myers, and Posa, 2001a)

$$0 < K_j \leq 1/\max\{\text{sill}(\gamma_j(\mathbf{h}_s, 0)); \text{sill}(\gamma_j(\mathbf{0}, h_t))\}. \tag{4}$$

In the application to the LCM the  $K_j$ 's are selected in such a way so as to ensure that the global sills are related to the sills for the different scales.

From (1) it follows that the spatial and temporal marginal matrix variograms for the LCM can be written, respectively, as

$$\mathbf{G}(\mathbf{h}_s, 0) = \sum_{j=1}^P \gamma_j(\mathbf{h}_s, 0) \mathbf{B}_j \tag{5}$$

$$\mathbf{G}(\mathbf{0}, h_t) = \sum_{j=1}^P \gamma_j(\mathbf{0}, h_t) \mathbf{B}_j. \tag{6}$$

Thus the space–time LCM is determined by two LCM’s, one is the space marginal and the other is the time marginal. This is analogous to the univariate case except that the coefficients are matrices.

### THE FITTING PROCESS

Initially the process of fitting is the same as in the usual process of fitting a LCM, the variation is that it must be done twice, once for the marginal time LCM and once for the marginal space LCM and with the constraint that the positive definite coefficient matrices are the same for both. For a spatial LCM it is necessary to determine the variograms of the uncorrelated components (and their number) and the coefficient matrices. For the extension to space–time using product–sum models, it is necessary to determine the marginals for each of the uncorrelated components, the coefficient matrices, and also the weights  $K_j$ ,  $j = 1, \dots, P$ . Note that the diagonal elements of the matrices defined in (5) and (6) are, respectively,

$$g_{ii}(\mathbf{h}_s, 0) = \sum_{j=1}^P b_{ii}^j(\mathbf{h}_s, 0), \quad i = 1, \dots, m, \quad (7)$$

$$g_{ii}(\mathbf{0}, h_t) = \sum_{j=1}^P b_{ii}^j(\mathbf{0}, h_t), \quad i = 1, \dots, m, \quad (8)$$

while the off-diagonal elements of the matrices defined in (5) and (6) are, respectively,

$$g_{ik}(\mathbf{h}_s, 0) = \sum_{j=1}^P b_{ik}^j(\mathbf{h}_s, 0), \quad i, j = 1, \dots, m, \quad i \neq k, \quad (9)$$

$$g_{ik}(\mathbf{0}, h_t) = \sum_{j=1}^P b_{ik}^j(\mathbf{0}, h_t), \quad i, j = 1, \dots, m, \quad i \neq k. \quad (10)$$

The fitting process uses some of the same techniques as in the purely spatial case.

- The first step is to compute the sample marginal space and marginal time variograms separately for each choice of  $i = 1, \dots, m$ . For each  $i$ ,  $A_i$  denotes the set of data locations in space–time for variable  $Z_i$ , then

$$\widehat{g}_{ii}(\mathbf{r}_{s_i}, 0) = \frac{1}{2|N_i(\mathbf{r}_{s_i})|} \sum_{N_i(\mathbf{r}_{s_i})} [Z_i(\mathbf{s} + \mathbf{h}_s, t) - Z_i(\mathbf{s}, t)]^2, \quad i = 1, \dots, m \quad (11)$$

$$\widehat{g}_{ii}(\mathbf{0}, r_{t_i}) = \frac{1}{2|M_i(r_{t_i})|} \sum_{M_i(r_{t_i})} [Z_i(\mathbf{s}, t + h_t) - Z_i(\mathbf{s}, t)]^2, \quad i = 1, \dots, m \quad (12)$$

where  $\mathbf{r}_{s_i}$  and  $r_{t_i}$  are, respectively, the vector lag with spatial tolerance  $s_i$  and the lag with temporal tolerance  $t_i$ .  $|N_i(\mathbf{r}_{s_i})|$  and  $|M_i(r_{t_i})|$  are the cardinalities of the following sets:

$$N_i(\mathbf{r}_{s_i}) = \{(\mathbf{s} + \mathbf{h}_s, t) \in A_i, (\mathbf{s}, t) \in A_i: \|\mathbf{r}_{s_i} - \mathbf{h}_s\| < s_i\}, \quad i = 1, \dots, m$$

$$M_i(r_{t_i}) = \{(\mathbf{s}, t + h_t) \in A_i, (\mathbf{s}, t) \in A_i: \|r_{t_i} - h_t\| < t_i\}, \quad i = 1, \dots, m.$$

- Fit nested variogram models  $g_{ii}(\mathbf{h}_s, 0)$  and  $g_{ii}(\mathbf{0}, h_t)$ ,  $i = 1, \dots, m$  to the sample variograms defined in (11) and (12). The model types and range parameters for all the marginal space variograms must be the same. The model types and the range parameters for all the marginal time variograms must be the same (but not necessarily the same as for the marginal space variograms). Moreover, the number of model types must be the same for the marginal space and marginal time variograms. Thus the  $g_{ii}(\mathbf{h}_s, 0)$ ,  $i = 1, \dots, m$  and the  $g_{ii}(\mathbf{0}, h_t)$ ,  $i = 1, \dots, m$ , are determined. Note that although modeled separately, for fixed  $j$  the coefficients  $b_{ii}^j$  are common to the marginal space and time variograms for each  $i$ .
- It is important to remember that the number of structures used in the LCM, i.e.,  $P$ , is the same for all  $i = 1, \dots, m$  and also the same for both the space marginals and the time marginals.
- In order to model  $g_{ii}(\mathbf{h}_s, h_t)$ ,  $i = 1, \dots, m$ , it is first necessary to complete the modeling of the  $g_j(\mathbf{h}_s, h_t)$ ,  $j = 1, \dots, P$ , that is, the  $K_j$ 's for  $j = 1, \dots, P$  must be determined. By considering the sample variogram surfaces  $\widehat{g}_{ii}(\mathbf{r}_{s_i}, r_{t_i})$ ,  $i = 1, \dots, m$ ,

$$\widehat{g}_{ii}(\mathbf{r}_{s_i}, r_{t_i}) = \frac{1}{2|V_{ii}(\mathbf{r}_{s_i}, r_{t_i})|} \sum_{V_{ii}(\mathbf{r}_{s_i}, r_{t_i})} [Z_i(\mathbf{s} + \mathbf{h}_s, t + h_t) - Z_i(\mathbf{s}, t)]^2 \quad (13)$$

where  $|V_{ii}(\mathbf{r}_{s_i}, r_{t_i})|$  is the cardinality of the set  $V_{ii}(\mathbf{r}_{s_i}, r_{t_i})$ , that is,

$$V_{ii}(\mathbf{r}_{s_i}, r_{t_i}) = \{(\mathbf{s} + \mathbf{h}_s, t + h_t) \in A_i, (\mathbf{s}, t) \in A_i: \|\mathbf{r}_{s_i} - \mathbf{h}_s\| < s_i, \|r_{t_i} - h_t\| < t_i\},$$

each constant,  $K_j$ , can be evaluated graphically or by estimating the global sill  $C_j(\mathbf{0}, 0) = sill(g_j(\mathbf{h}_s, h_t))$ .

- To complete the LCM product–sum space–time model it is only necessary to determine the coefficients  $b_{ik}^j, i \neq k$ , i.e., the off-diagonal entries in the  $\mathbf{B}_j$ 's,  $j = 1, \dots, P$ . These will then determine the space–time cross-variograms since all other terms in the marginal space cross-variograms and the marginal time cross-variograms (9) and (10) have already been determined. Moreover the  $K_j$ 's have already been computed. The off-diagonal entries must be chosen to ensure that each  $\mathbf{B}_j$  is positive definite or at least nonnegative definite.
- Compute the sample marginal spatial and temporal cross-variograms corresponding to  $g_{ik}(\mathbf{h}_s, 0)$  and  $g_{ik}(\mathbf{0}, h_t)$ , defined in (9) and (10), respectively:

$$\widehat{g}_{ik}(\mathbf{r}_{s_{ik}}, 0) = \frac{1}{2|Q_{ik}(\mathbf{r}_{s_{ik}})|} \sum_{Q_{ik}(\mathbf{r}_{s_{ik}})} [Z_i(\mathbf{s} + \mathbf{h}_s, t) - Z_i(\mathbf{s}, t)][Z_k(\mathbf{s} + \mathbf{h}_s, t) - Z_k(\mathbf{s}, t)], \quad (14)$$

$$\widehat{g}_{ik}(\mathbf{0}, r_{t_{ik}}) = \frac{1}{2|T_{ik}(r_{t_{ik}})|} \sum_{T_{ik}(r_{t_{ik}})} [Z_i(\mathbf{s}, t + h_t) - Z_i(\mathbf{s}, t)][Z_k(\mathbf{s}, t + h_t) - Z_k(\mathbf{s}, t)], \quad (15)$$

where  $\mathbf{r}_{s_{ik}}$  and  $r_{t_{ik}}$  are, respectively, the vector lag with spatial tolerance  $s_{ik}$  and the lag with temporal tolerance  $t_{ik}$ .  $|Q_{ik}(\mathbf{r}_{s_{ik}})|$  and  $|T_{ik}(r_{t_{ik}})|$  are the cardinalities of the following sets:

$$Q_{ik}(\mathbf{r}_{s_{ik}}) = \{(\mathbf{s} + \mathbf{h}_s, t) \in A_i \cap A_k, (\mathbf{s}, t) \in A_i \cap A_k: \|\mathbf{r}_{s_{ik}} - \mathbf{h}_s\| < s_{ik}\},$$

$$T_{ik}(r_{t_{ik}}) = \{(\mathbf{s}, t + h_t) \in A_i \cap A_k, (\mathbf{s}, t) \in A_i \cap A_k: \|r_{t_{ik}} - h_t\| < t_{ik}\}.$$

### Evaluating the Model Fit

The ultimate objective is to fit the space–time LCM, given in Eq. (1). The simplest approach is to evaluate the fit of the space and time marginals, but there are at least two more ways to evaluate the fit.

1. Apply cross-validation with cokriging in space–time. There are several difficulties and drawbacks to this. One problem is that one obtains not one “error” (the difference between the observed data value and the estimated value) but rather one for each variable. Thus, there is a set of cross-validation statistics for each variable or one must construct a composite statistic. The former may result in too much information and make it difficult to discern where any problem occurs. The latter may cover up

inadequate modeling of variograms and cross-variograms for only some of the variables.

2. Compute a mean square metric corresponding to the difference between the sample matrix variogram and the fitted model. For each lag this difference will be a matrix and hence one must use a metric, e.g., the usual matrix norm. This might be written in the following form:

$$\sum_{(\mathbf{h}_s, h_t)} \frac{\|\widehat{G}(\mathbf{h}_s, h_t) - G(\mathbf{h}_s, h_t)\|^2}{\|G(\mathbf{h}_s, h_t)\|^2}.$$

### A CASE STUDY

The spatiotemporal data set used for illustrating the proposed methodology consists of hourly averages values of NO<sub>2</sub> and CO measured over Milan district at 54 and 31 monitoring stations, respectively, during February 1999.

Let

$$\mathbf{Z}(\mathbf{s}, t) = [Z_1(\mathbf{s}, t), Z_2(\mathbf{s}, t)]^T$$

where  $Z_1$  and  $Z_2$  are the hourly average values of CO and NO<sub>2</sub>, respectively. The monitoring station locations are shown in Figure 1. Note from Figure 1 that the set of the monitoring data locations for CO is a subset of the set of the monitoring data locations for NO<sub>2</sub>.

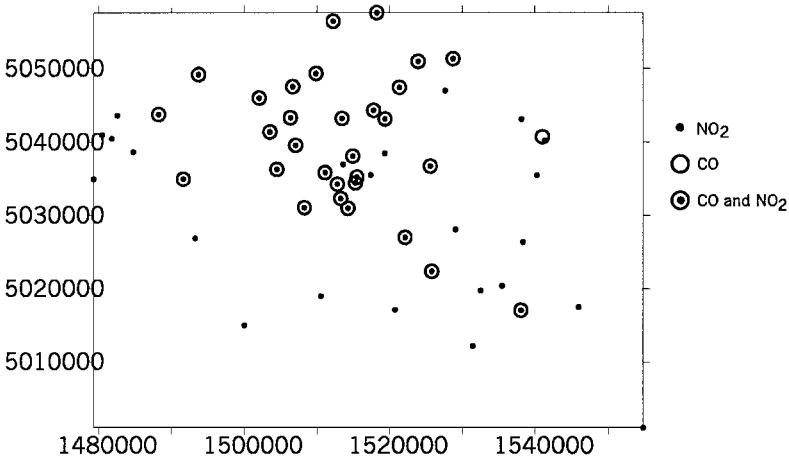


Figure 1. Posting map of the survey stations for CO and NO<sub>2</sub> in the Milan district.

### Modeling the Marginal Variograms

The set of data locations in space–time for CO ( $i = 1$ ) and NO<sub>2</sub> ( $i = 2$ ), respectively, are:

$$A_i = ((s_k, t_j), k = 1, 2, \dots, n_i, j = 1, 2, \dots, 672), \quad i = 1, 2,$$

where the monitoring stations are  $n_1 = 31$  CO and  $n_2 = 54$ , for NO<sub>2</sub>, and a time series of 672 hourly average values (corresponding to 28 days of February) is available at each spatial location.

Figures 2(a) and (b) show the sample marginal variograms for space and time of both variables, where the continuous curves represent the fitted models. For simplicity, the model types are given in abbreviated form as follows:

1.  $\text{sph}(r/a)$  is an isotropic spherical unit *sill* model with range  $a$ ;
2.  $\text{exp}(r/a)$  is an isotropic exponential unit *sill* model with *effective* range  $a$ , i.e., the distance needed to reach 95% of the *sill* value;
3.  $\text{cos}(r/a)$  is an isotropic cosine model with period  $a$ . Although the cosine model would be only semidefinite, when nested with a (conditionally negative) definite model the result is a valid variogram model. This model is only used with the temporal marginal variograms.

The analytic forms of the fitted models for CO hourly averages, are

$$g_{11}(\mathbf{h}_s, 0) = 0.75 \text{ }_1(\mathbf{h}_s, 0) + 0.31 \text{ }_2(\mathbf{h}_s, 0) + 0.33 \text{ }_3(\mathbf{h}_s, 0) \quad (16)$$

where

$$\text{ }_1(\mathbf{h}_s, 0) = \begin{cases} 0 & \|\mathbf{h}_s\| = 0 \\ 1 & \|\mathbf{h}_s\| > 0 \end{cases} \quad (17)$$

$$\text{ }_2(\mathbf{h}_s, 0) = \text{sph}\left(\frac{\|\mathbf{h}_s\|}{7}\right) \quad (18)$$

$$\text{ }_3(\mathbf{h}_s, 0) = \text{exp}\left(\frac{\|\mathbf{h}_s\|}{15}\right) \quad (19)$$

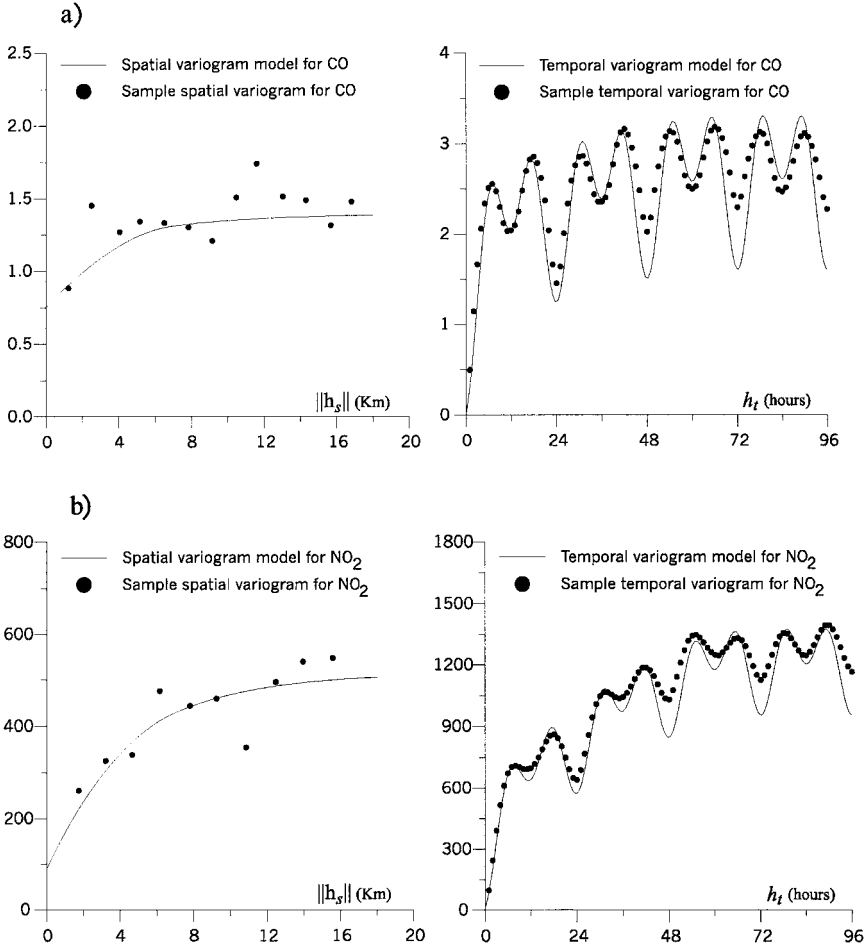
where the spatial distances in (18) and in (19) are given in kilometers, and

$$g_{11}(\mathbf{0}, h_t) = 0.75 \text{ }_1(\mathbf{0}, h_t) + 0.31 \text{ }_2(\mathbf{0}, h_t) + 0.33 \text{ }_3(\mathbf{0}, h_t) \quad (20)$$

where

$$\text{ }_1(\mathbf{0}, h_t) = \begin{cases} 0 & h_t = 0 \\ 0.01 & h_t > 0 \end{cases} \quad (21)$$





**Figure 2.** Sample marginal variograms for space and time of (a) CO and their models and (b) NO<sub>2</sub> and their models.

$${}_2(\mathbf{0}, h_t) = 2.92 \exp\left(\frac{h_t}{12}\right) + 1.86 \cos\left(\frac{h_t}{12}\right) + 1.62 \cos\left(\frac{h_t}{24}\right) \quad (22)$$

$${}_3(\mathbf{0}, h_t) = 2.1 \text{ sph}\left(\frac{h_t}{72}\right). \quad (23)$$

Likewise for NO<sub>2</sub> hourly averages, the marginal variograms are

$$g_{22}(\mathbf{h}_s, 0) = 90 \quad {}_1(\mathbf{h}_s, 0) + 75.38 \quad {}_2(\mathbf{h}_s, 0) + 350 \quad {}_3(\mathbf{h}_s, 0) \quad (24)$$

where  $\gamma_i(\mathbf{h}_s, 0), i = 1, \dots, 3$  were defined in (17), (18), and (19), and

$$g_{22}(\mathbf{0}, h_t) = 90 \gamma_1(\mathbf{0}, h_t) + 75.38 \gamma_2(\mathbf{0}, h_t) + 350 \gamma_3(\mathbf{0}, h_t), \quad (25)$$

where  $\gamma_i(\mathbf{0}, h_t), i = 1, \dots, 3$  were defined in (21), (22), and (23).

Note that the number of basic components in the marginal space and time variograms is the same for both variables. Moreover both marginal variograms are represented in terms of the same basic components.

As regards the interpretation of the above variogram models, it can be said that they recall the experimental variogram features, such as nugget effect, periodicity, and range. Particularly, the two temporal periodicities at 12 and 24 h might be linked to the cycle of factors which influence pollution, such as human activities, sunlight effects, and photochemical reactions.

### Estimation of $K_j$ 's of the Product–Sum Nested Models

The structural analysis is completed by estimating the coefficients  $K_j, j = 1, 2, 3$  of the space–time nested models. They have been estimated graphically by comparing the sample variogram surfaces with the product–sum models (Fig. 3). The best fits are obtained with  $K_1 = 0.45, K_2 = 0.02,$  and  $K_3 = 0.33$ .

### Marginal Cross-Variogram Models

In this case study, since there are only two variables, to complete the space–time LCM it is necessary to determine only one off diagonal entry in each  $B_j, j = 1, 2, 3$  (each coefficient matrix is symmetric). These off diagonal entries must be chosen so that each  $B_j, j = 1, 2, 3$  is positive definite (or at least semidefinite). Obviously the resulting cross-variogram models should “fit” the data. Since there are only three unknown entries to be determined, this was done partly by trial and error using the sample marginal space and time cross-variograms (Fig. 4). More general methods would have to be used if  $P$  is larger and/or there are more than two variables. The fitted models are shown in Figure 4 and the analytic forms are

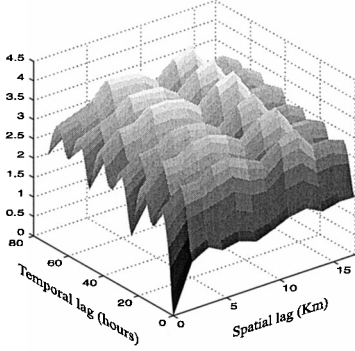
$$g_{12}(\mathbf{h}_s, 0) = 0 \gamma_1(\mathbf{h}_s, 0) + 3.08 \gamma_2(\mathbf{h}_s, 0) + 11.67 \gamma_3(\mathbf{h}_s, 0) \quad (26)$$

where  $\gamma_i(\mathbf{h}_s, 0), i = 1, \dots, 3$  were defined in (17), (18), and (19), and

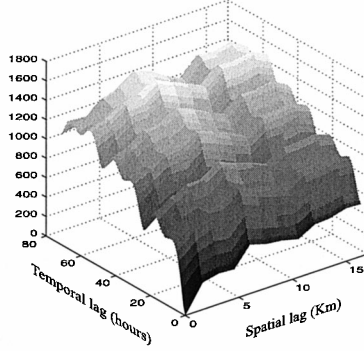
$$g_{12}(\mathbf{0}, h_t) = 0 \gamma_1(\mathbf{0}, h_t) + 3.08 \gamma_2(\mathbf{0}, h_t) + 11.67 \gamma_3(\mathbf{0}, h_t) \quad (27)$$

where  $\gamma_i(\mathbf{0}, h_t), i = 1, \dots, 3$  were defined in (21), (22), and (23).

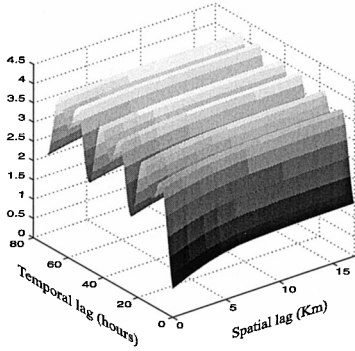
a) Sample spatial–temporal variogram for CO



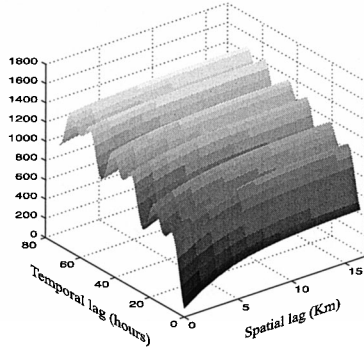
Sample spatial–temporal variogram for NO<sub>2</sub>



b) Spatial–temporal variogram model for CO



Spatial–temporal variogram model for NO<sub>2</sub>



Figure

3. (a) Sample variogram surfaces of CO and NO<sub>2</sub>; (b) their space–time models with  $K_1 = 0.45$ ,  $K_2 = 0.02$ , and  $K_3 = 0.33$ .

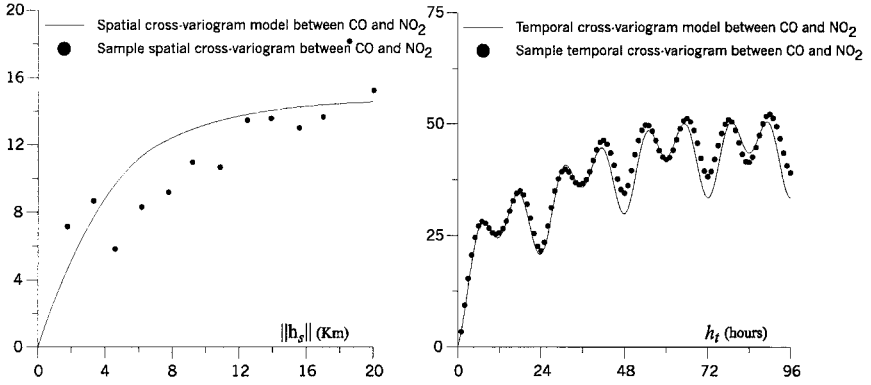
### The Fitted Space–Time LCM

The space–time LCM can be determined using (1):

$$\mathbf{G}(\mathbf{h}_s, h_t) = {}_1(\mathbf{h}_s, h_t) \mathbf{B}_1 + {}_2(\mathbf{h}_s, h_t) \mathbf{B}_2 + {}_3(\mathbf{h}_s, h_t) \mathbf{B}_3. \quad (28)$$

From the previous sections, the matrices  $B_j, j = 1, \dots, 3$  are

$$\mathbf{B}_1 = \begin{bmatrix} 0.75 & 0 \\ 0 & 90 \end{bmatrix}, \quad \mathbf{B}_2 = \begin{bmatrix} 0.31 & 3.08 \\ 3.08 & 75.38 \end{bmatrix}, \quad \mathbf{B}_3 = \begin{bmatrix} 0.33 & 11.67 \\ 11.67 & 350 \end{bmatrix}$$



**Figure 4.** Sample marginal cross-variograms between CO and NO<sub>2</sub> for space and time and their models.

To complete the space–time LCM (1) it is necessary to construct, for each  $j = 1, \dots, 3$ , the  $\gamma_j(\mathbf{h}_s, h_t)$ 's using the respective marginals  $\gamma_j(\mathbf{h}_s, 0)$ ,  $\gamma_j(\mathbf{0}, h_t)$  and the value of  $K_j$  using (2):

$$\gamma_1(\mathbf{h}_s, h_t) = \gamma_1(\mathbf{h}_s, 0) + \gamma_1(\mathbf{0}, h_t) - 0.45 \gamma_1(\mathbf{h}_s, 0) \gamma_1(\mathbf{0}, h_t)$$

where  $\gamma_1(\mathbf{h}_s, 0)$  is given in Eq. (17) and  $\gamma_1(\mathbf{0}, h_t)$  is given in Eq. (21);

$$\gamma_2(\mathbf{h}_s, h_t) = \gamma_2(\mathbf{h}_s, 0) + \gamma_2(\mathbf{0}, h_t) - 0.02 \gamma_2(\mathbf{h}_s, 0) \gamma_2(\mathbf{0}, h_t)$$

where  $\gamma_2(\mathbf{h}_s, 0)$  is given in Eq. (18) and  $\gamma_2(\mathbf{0}, h_t)$  is given in Eq. (22);

$$\gamma_3(\mathbf{h}_s, h_t) = \gamma_3(\mathbf{h}_s, 0) + \gamma_3(\mathbf{0}, h_t) - 0.33 \gamma_3(\mathbf{h}_s, 0) \gamma_3(\mathbf{0}, h_t)$$

where  $\gamma_3(\mathbf{h}_s, 0)$  is given in Eq. (19) and  $\gamma_3(\mathbf{0}, h_t)$  is given in Eq. (23).

### FURTHER RESULTS ON FITTING SPACE–TIME LCMs

As noted in the Introduction section, the LCM corresponds to the assumption that the matrix variogram can be diagonalized. In fact, (1) can be written as

$$\mathbf{G}(\mathbf{h}_s, h_t) = \mathbf{D} \text{diag}(\gamma_1(\mathbf{h}_s, h_t), \dots, \gamma_p(\mathbf{h}_s, h_t)) \mathbf{D}^T.$$

If the basic structures  $\gamma_1(\mathbf{h}_s, h_t), \dots, \gamma_p(\mathbf{h}_s, h_t)$  are known, then fitting the model corresponds to finding the matrix  $\mathbf{D}$  which will “diagonalize” the model. The

columns of  $\mathbf{D}$  will determine all the  $B_j$ 's,  $\mathbf{D}$  will generally not be square and does not have to satisfy a positive definiteness condition. The entries in  $\mathbf{D}$  might be determined by a least squares fit to the sample spatial–temporal variogram matrix. This is similar to the approach proposed by Goulard and Voltz (1992). Alternatively, if the marginal basic structures are known, i.e., have already been determined, then the diagonalized form of these could be simultaneously fit to the sample marginal variogram matrices. Xie and Myers (1995) and Xie, Myers, and Long (1995) propose a slightly different approach that could be extended to the space–time problem.

### SUMMARY

The LCM for a matrix variogram can be generalized to incorporate space–time modeling. It has been shown that by using the product–sum variogram, the space and time marginals can be adopted to fit the space–time variogram in the LCM.

More general models can be constructed by assuming integrated product or integrated product–sum models as basic structures, instead of product–sum models. The method utilized in De Iaco, Myers, and Posa (2002) might then be used to fit the probability distribution. The simplest form would be to assume that the same distribution is used in all the integrated models.

An application to an air pollution data set is given.

### REFERENCES

- Bilonick, R. A., 1985, The space–time distribution of sulfate deposition in the Northeastern United States: *Atmos. Environ.*, v. 19, no. 11, p. 1829–1845.
- Christakos, G., 1992, *Random field models in earth sciences*: Academic Press, New York, 474 p.
- De Cesare, L., Myers, D., and Posa, D., 2001a, Product–sum covariance for space–time modeling: *Environmetrics*, v. 12, p. 11–23.
- De Cesare, L., Myers, D., and Posa, D., 2001b, Estimating and modeling space–time correlation structures: *Stat. Prob. Lett.*, v. 51, no. 1, p. 9–14.
- De Cesare, L., Myers, D., and Posa, D., 2002, FORTRAN 77 programs for space–time modeling: *Comput. Geosci.*, v. 28, no. 2, p. 205–212.
- De Iaco, S., Myers, D., and Posa, D., 2001a, Space–time analysis using a general product–sum model: *Stat. Prob. Lett.*, v. 52, no. 1, p. 21–28.
- De Iaco, S., Myers, D., and Posa, D., 2001b, Total air pollution and space–time modeling, *in* Monestiez, P., Allard, D., and Froidevaux, R., eds., *geoENV III, Geostatistics for environmental applications*: Kluwer, Dordrecht, The Netherlands, p. 45–56.
- De Iaco, S., Myers, D., and Posa, D., 2002, Nonseparable space–time covariance models: Some parametric families: *Math. Geol.*, v. 34, no. 1, p. 23–41.
- Goovaerts, P., 1993, Spatial orthogonality of the principal components computed from coregionalized variables: *Math. Geol.*, v. 25, no. 3, p. 281–302.

- Goovaerts, P., and Sonnet, Ph., 1993, Study of spatial and temporal variations of hydrogeochemical variables using factorial kriging analysis, *in* Soares, A., ed., *Geostatistics Troia '92*: Kluwer, Dordrecht, The Netherlands, v. 2, p. 745–756.
- Goulard, M., and Voltz, M., 1992, Linear coregionalization model: Tools for estimation and choice of cross-variogram matrix: *Math. Geol.*, v. 24, no. 3, p. 269–286.
- Journel, A. G., and Huijbregts, C. J., 1981, *Mining geostatistics*: Academic Press, London, 595 p.
- Kyriakidis, P. C., and Journel, A. G., 1999, Geostatistical space–time models: A review: *Math. Geol.*, v. 31, no. 6, p. 651–684.
- Rouhani, S., and Wackernagel, H., 1990, Multivariate geostatistical approach to space–time data analysis: *Water Resour. Res.*, v. 26, p. 585–591.
- Xie, T., and Myers, D. E., 1995, Fitting matrix valued variogram models by simultaneous diagonalization I: Theory: *Math. Geol.*, v. 27, no. 7, p. 867–876.
- Xie, T., Myers, D. E., and Long, A. E., 1995, Fitting matrix valued variogram models by simultaneous diagonalization, II: Applications, *Math. Geol.*, v. 27, no. 7, p. 877–888.