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Nonseparable Space-Time Covariance Models: Some Parametric Families[1]

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By extending the product and product–sum space-time covariance models, new families are generated as integrated products and product–sums. These include nonintegrable space-time covariance models not obtainable by the Cressie–Huang representation. It is shown how to fit the spatial and temporal components of the models as well as the probability density function. The methods are illustrated by a case study.

KEY WORDS: product–sum models, integrated models, separability, admissibility.

INTRODUCTION

While there are no difficulties in extending the various kriging estimators and the kriging equations to the space-time setting, there has been a lack of known valid space-time covariances and variograms. The obvious possibility for extending to space-time involves the use of a zonal anisotropy: the difficulties associated with this method are discussed in Myers and Journel (1990) and Rouhani and Myers (1990). A recent review of geostatistical space-time models was given by Kyriakidis and Journel (1999).

In order to estimate the correlation of a space-time process, the main questions are as follows:

- Is it useful and does it make sense to define a spatio-temporal metric, such as

$$d(\mathbf{u_1}, \mathbf{u_2}) = (a(x_1 - x_2)^2 + b(y_1 - y_2)^2 + c(t_1 - t_2)^2)^{1/2},$$

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with $\mathbf{u_1} = (x_1, y_1, t_1)$, $\mathbf{u_2} = (x_2, y_2, t_2)$, where $(x_1, y_1), (x_2, y_2) \in D \subseteq \Re^2$, and $t_1, t_2 \in T \subseteq \Re$, where D and T are the spatial and temporal domains, respectively. In general the units for space and time will be disparate, e.g., meters and hours.

- How to choose a space-time covariance or variogram model and how to choose parameters to ensure that the best fit to data is achieved?

One of the objectives of this paper is to furnish answers to the above questions; moreover, starting from the product–sum covariance model (De Cesare, Myers, and Posa, 2001) and by using the stability properties, some nonseparable parametric families of space-time covariance functions have been derived. It is important to point out that this new class of models cannot be obtained, in general, from the Cressie–Huang representation (Cressie and Huang, 1999).

SOME PARAMETRIC FAMILIES OF SPACE-TIME STATIONARY COVARIANCES

Most space-time covariance or variogram models, in literature, have been derived by utilizing the following theoretical results, since covariances or variograms in $\Re^n$ can be obtained, in general, from other valid functions.

1. From the *convexity property* of the family of covariances, if $C_1(\mathbf{h})$ and $C_2(\mathbf{h})$ are covariances in $\Re^n$ and $b > 0$, then both $C_1(\mathbf{h}) + C_2(\mathbf{h})$ and $b \cdot C_1(\mathbf{h})$ are covariances in $\Re^n$. The same results hold for the family of variograms.
2. From the *first stability property* (Chilès and Delfiner, 1999, p. 60), if $C_1(\mathbf{h})$ and $C_2(\mathbf{h})$ are covariances in $\Re^n$, then their product, $C_1(\mathbf{h}) \cdot C_2(\mathbf{h})$, is still a covariance in $\Re^n$.
3. From the *second stability property* (Chilès and Delfiner, 1999), if $\mu(a)$ is a positive measure in $U \subseteq \Re$ and $C(\mathbf{x}, \mathbf{y}; a)$ is a covariance function in $\Re^n$ for each $a \in V \subseteq U$, which is integrable over the subset V of U for every pair $(\mathbf{x}, \mathbf{y})$, then $C(\mathbf{x}, \mathbf{y})$, defined as

$$C(\mathbf{x}, \mathbf{y}) = \int_V C(\mathbf{x}, \mathbf{y}; a)\, d\mu(a),$$

   is a covariance in $\Re^n$ (Matern, 1980, p. 10).
4. Representing the random field in $\Re^n$ as a combination of independent components in the separate domains, one can utilize the following separable models:

   a) the *factorized or separable covariance* (Chilès and Delfiner, 1999):

$$C(\mathbf{h}) = \prod_{i=1}^{n} C_i(h_i), \tag{1}$$

where $Z(\mathbf{u}) = \prod_{i=1}^{n} Z_i(u_i)$ and the Z_i's are uncorrelated random fields in $\Re$;

b) the *nested structure variogram*:

$$\gamma(\mathbf{h}) = \sum_{i=1}^{n} \gamma_i(h_i), \tag{2}$$

where $Z(\mathbf{u}) = \sum_{i=1}^{n} Z_i(u_i)$ and the Z_i's are uncorrelated random fields in $\Re$.

In both cases h_i are the components of the vector $\mathbf{h}$ and $C_i(h_i)$ and $\gamma_i(h_i)$ are, respectively, covariances and variograms in $\Re$, $i = 1, \ldots, n$.

Hence, under the convenient assumption of treating space and time separately, the factorized covariance (1) and the nested variogram (2) represent one of the first attempts to generate parametric families of space-time covariances and variograms. The product model (De Cesare, Myers, and Posa, 1997; Posa, 1993; Rodriguez-Iturbe and Mejia, 1974) and the nested model (Rouhani and Hall, 1989) belong to this category. The nested model will in general not be strictly positive definite but only semidefinite (Myers and Journel, 1990).

The Product–Sum Covariance Model

An extension of these two simple models (product model and nested model) is given by the class of product–sum covariance models, introduced in De Cesare, Myers, and Posa (2001):

$$C_{\mathrm{s,t}}(\mathbf{h}_{\mathrm{s}}, h_{\mathrm{t}}) = k_1 C_{\mathrm{s}}(\mathbf{h}_{\mathrm{s}}) C_{\mathrm{t}}(h_{\mathrm{t}}) + k_2 C_{\mathrm{s}}(\mathbf{h}_{\mathrm{s}}) + k_3 C_{\mathrm{t}}(h_{\mathrm{t}}), \tag{3}$$

where C_{t} and C_{s} are valid temporal and spatial covariance models, respectively. Note that these models are generally nonseparable.

Cressie–Huang Models

Cressie and Huang (1999) have recently shown how to construct some non-separable classes of integrable space-time covariances. They used the representation:

$$C_{\mathrm{s,t}}(\mathbf{h}_{\mathrm{s}}, h_{\mathrm{t}}) = \int_{\Re^n} e^{i\mathbf{h}_{\mathrm{s}}'\omega} \rho(\omega; h_{\mathrm{t}}) k(\omega)\, d\omega,$$

where $\rho(\omega;\cdot)$ is a continuous autocorrelation function for each $\omega \in \Re^n$,

$$\int_{\Re_+} \rho(\omega; h_t)\, dh_t < \infty,$$

$$k(\omega) > 0 \quad \text{and} \quad \int_{\Re^n} k(\omega)\, d\omega < \infty.$$

These spatial–temporal covariances are generated by using Bochner's theorem and by choosing an appropriate spectral density.

NEW PARAMETRIC FAMILIES OF SPACE-TIME COVARIANCE MODELS

Both the product–sum and the Cressie–Huang constructions will now be extended.

Theorem 1. *Let $\mu(a)$ be a positive measure over $U \subseteq \Re$, let $C_s(\mathbf{h}_s; a)$ and $C_t(h_t; a)$ be covariances, respectively, in $D \subset \Re^n$ and $T \subset \Re_+$, for each $a \in V \subseteq U$.*

(a) *If $C_s(\mathbf{h}_s; a) \cdot C_t(h_t; a)$ is integrable with respect to the measure μ over V for each $\mathbf{h}_s$ and h_t, given $k > 0$, then*

$$C_{s,t}(\mathbf{h}_s, h_t) = \int_V k C_s(\mathbf{h}_s; a) C_t(h_t; a)\, d\mu(a) \tag{4}$$

is a covariance in $D \times T$.

(b) *Likewise, if $k_1 C_s(\mathbf{h}_s; a) C_t(h_t; a) + k_2 C_s(\mathbf{h}_s; a) + k_3 C_t(h_t; a)$ is integrable with respect to the measure μ over V for each $\mathbf{h}_s$ and h_t, given $k_1 > 0$, $k_2 \geq 0$, and $k_3 \geq 0$, then*

$$C_{s,t}(\mathbf{h}_s, h_t) = \int_V [k_1 C_s(\mathbf{h}_s; a) C_t(h_t; a) + k_2 C_s(\mathbf{h}_s; a) + k_3 C_t(h_t; a)]\, d\mu(a) \tag{5}$$

is a covariance in $D \times T$.

This result follows from the second stability property and the previous models, such as the product and product–sum covariance models. Since the product and the product–sum covariance models can be written in terms of the variograms (De Cesare, Myers, and Posa, 1997, 2001), from Theorem 1 it follows that

$$\gamma_{s,t}(\mathbf{h}_s, h_t) = \int_V k[C_t(0; a)\gamma_s(\mathbf{h}_s; a) + C_s(\mathbf{0}; a)\gamma_t(h_t; a) - \gamma_s(\mathbf{h}_s; a)\gamma_t(h_t; a)]\, d\mu(a), \tag{6}$$

and

$$\gamma_{s,t}(\mathbf{h}_s, h_t) = \int_V [(k_2 + k_1 C_t(0; a))\gamma_s(\mathbf{h}_s; a) + (k_3 + k_1 C_s(\mathbf{0}; a))\gamma_t(h_t; a) - k_1 \gamma_s(\mathbf{h}_s; a)\gamma_t(h_t; a)]\, d\mu(a), \tag{7}$$

where $\gamma_s(\mathbf{h}_s; a)$ and $\gamma_t(h_t; a)$ are valid spatial and temporal variogram models for each choice of $a \in V$, while $C_s(\mathbf{0}; a)$ and $C_t(0; a)$ are the corresponding sill values.

Remarks.

- In general product–sum covariance models are not integrable over $\mathbf{h}_s$ and h_t, are not separable, and do not correspond to the use of a space-time metric. Models obtained by an integrated product–sum representation will have the same characteristics.
- Although the product covariance models are separable and integrable, the integrated product representation (4) can also produce nonseparable and nonintegrable models, as will be shown in the following examples. Hence, this new class of models cannot be obtained, in general, from the Cressie–Huang representation.
- Since the complex exponential can be written as

$$e^{i\mathbf{h}'\omega} = \cos(\mathbf{h}'\omega) + i\ \sin(\mathbf{h}'\omega)$$

if $\rho(\omega; h_t)k(\omega)$ is symmetric about the origin in $\Re^n$, then Cressie–Huang representation can be viewed as a special case of (4). Hence,

$$C_{s,t}(\mathbf{h}_s, h_t) = \int_{\Re^n} e^{i\mathbf{h}_s'\omega} \rho(\omega; h_t)k(\omega)\, d\omega = \int_{\Re_+^n} C_s(\mathbf{h}_s; \omega)C_t(h_t; \omega)k(\omega)\, d\omega,$$

where $k(\omega)$ is defined, positive, and integrable over $\Re_+^n = \Re_+ \times \cdots \times \Re_+$ n times; $C_s(\mathbf{h}_s; \omega)$ is only a positive semidefinite spatial covariance function for each $\omega \in \Re_+^n$; and $C_t(h_t; \omega)$ is a temporal covariance. In this special case only, the nonseparable Cressie–Huang covariance models could be rewritten in terms of variograms as in (6) and take advantage of the property that variograms are zero at zero lag. All the covariance models obtained by Cressie and Huang satisfy the symmetry property; moreover, $\gamma_{s,t}(\mathbf{h}_s, h_t)$, $\gamma_{s,t}(\mathbf{h}_s, 0)$, and $\gamma_{s,t}(\mathbf{0}, h_t)$ have the same sill values.
- By using nonseparable Cressie–Huang models, one could take into account separate space and time components only by adding them to the model considered, while in the above product–sum and the integrated product–sum

models, separate spatial and temporal structures are a part of the models by construction.

Obviously there are practical problems in choosing among the parametric families of variograms that can be generated from (6) and (7), one that is closest to the empirical space-time variogram. Both of these problems are considered later. In the following section, Theorem 1 is used to generate examples of parametric families of space-time covariance functions.

Some Examples

By applying Theorem 1, a wide class of parametric families of space-time covariance models are obtained. Suppose that the measure μ is generated by an absolutely continuous function Φ, then there exists a function ϕ such that $d\Phi(a) = \phi(a)\, da$ almost everywhere. The following examples, based on particular choices of isotropic covariances and functions ϕ, show that one can obtain other families by using the same hypothesis and criteria. The integrals considered in the following examples are easily evaluated (Gradshteyn and Ryzhik, 2000).

Example 1. Given the following functions:

$$C_{\mathrm{s}}(\mathbf{h}_{\mathrm{s}}; a, b, \alpha) = e^{-\frac{a\|\mathbf{h}_{\mathrm{s}}\|^{\alpha}}{b}}, \quad 1 \leq \alpha \leq 2,\ a > 0,\ b > 0,$$

$$C_{\mathrm{t}}(h_{\mathrm{t}}; a, c, \delta) = e^{-\frac{a h_{\mathrm{t}}^{\delta}}{c}}, \quad 1 \leq \delta \leq 2,\ c > 0,$$

$$\phi(a, n, \beta) = \frac{\beta^{n+1}}{\Gamma(n+1)}\, a^{n}\, e^{-\beta a}, \quad n \geq 0,\ \beta > 0,$$

since $C_{\mathrm{s}}(\mathbf{h}_{\mathrm{s}}; a, b, \alpha)$ and $C_{\mathrm{t}}(h_{\mathrm{t}}; a, c, \delta)$ are, respectively, valid spatial and temporal covariance models for each choice of a over the interval $V = [0; +\infty[$, the integrability conditions of Theorem 1 are satisfied and two new classes of nonseparable space-time covariances can be obtained:

$$\begin{aligned} C_{\mathrm{s,t}}(\mathbf{h}_{\mathrm{s}}, h_{\mathrm{t}}; \boldsymbol{\Theta}_{\mathbf{1}}) &= \int_{V} k\, e^{-\frac{a\|\mathbf{h}_{\mathrm{s}}\|^{\alpha}}{b}} \cdot e^{-\frac{a h_{\mathrm{t}}^{\delta}}{c}} \cdot \frac{\beta^{n+1}}{\Gamma(n+1)}\, a^{n}\, e^{-\beta a}\, da \\ &= \frac{k\beta^{n+1}}{\Gamma(n+1)} \int_{V} a^{n}\, e^{-a\left(\frac{\|\mathbf{h}_{\mathrm{s}}\|^{\alpha}}{b} + \frac{\mathbf{h}_{\mathrm{t}}^{\delta}}{c} + \beta\right)}\, da \\ &= \frac{k\beta^{n+1}}{\left(\frac{\|\mathbf{h}_{\mathrm{s}}\|^{\alpha}}{b} + \frac{h_{\mathrm{t}}^{\delta}}{c} + \beta\right)^{n+1}}, \end{aligned} \tag{8}$$

where $\mathbf{\Theta_1} = (b, c, n, k, \alpha, \beta, \delta)$;

$$C_{s,t}(\mathbf{h}_s, h_t; \mathbf{\Theta_2}) = \int_V \left[k_1\, e^{-\frac{a\|\mathbf{h}_s\|^\alpha}{b}} \cdot e^{-\frac{a h_t^\delta}{c}} + k_2\, e^{-\frac{a\|\mathbf{h}_s\|^\alpha}{b}} + k_3\, e^{-\frac{a h_t^\delta}{c}} \right] \times \frac{\beta^{n+1}}{\Gamma(n+1)}\, a^n\, e^{-\beta a}\, da$$
$$= k_1 \frac{\beta^{n+1}}{\left(\frac{\|\mathbf{h}_s\|^\alpha}{b} + \frac{h_t^\delta}{c} + \beta\right)^{n+1}} + k_2 \frac{\beta^{n+1}}{\left(\frac{\|\mathbf{h}_s\|^\alpha}{b} + \beta\right)^{n+1}} + k_3 \frac{\beta^{n+1}}{\left(\frac{h_t^\delta}{c} + \beta\right)^{n+1}}, \tag{9}$$

where $\mathbf{\Theta_2} = (b, c, n, k_1, k_2, k_3, \alpha, \beta, \delta)$.

Note that, when $\alpha = \delta = 1$ and $n = 0$, $(\frac{\|\mathbf{h}_s\|}{b} + \frac{h_t}{c})$ in (8) and (9) might correspond to a space-time metric and $\frac{\beta}{(\frac{\|\mathbf{h}_s\|^\alpha}{b} + \frac{h_t^\delta}{c} + \beta)}$ would belong to a well known family of covariance models, namely,

$$C(\mathbf{h}; w_1, w_2) = \frac{w_1}{w_2 + \|\mathbf{h}\|}.$$

Example 2. Given the functions

$$C_s(\mathbf{h}_s; a, b, \alpha) = e^{-\frac{a^2\|\mathbf{h}_s\|^\alpha}{b}}, \quad 1 \le \alpha \le 2,\ a > 0,\ b > 0,$$
$$C_t(h_t; a, c, \delta) = e^{-\frac{a^2 h_t^\delta}{c}}, \quad 1 \le \delta \le 2,\ c > 0,$$
$$\phi(a, n, \beta) = \frac{2\beta^{(n+1)/2}}{\Gamma((n+1)/2)}\, a^n\, e^{-\beta a^2}, \quad n \ge 0,\ \beta > 0,$$

since $C_s(\mathbf{h}_s; a, b, \alpha)$ and $C_t(h_t; a, c, \delta)$ are, respectively, valid spatial and temporal covariance models for each choice of a over the interval $V = [0; +\infty[$, the integrability conditions of Theorem 1 are satisfied and two new classes of nonseparable space-time covariances can be obtained:

$$C_{s,t}(\mathbf{h}_s, h_t; \mathbf{\Theta_1}) = \int_V k\, e^{-\frac{a^2\|\mathbf{h}_s\|^\alpha}{b}} \cdot e^{-\frac{a^2 h_t^\delta}{c}} \cdot \frac{2\beta^{(n+1)/2}}{\Gamma((n+1)/2)}\, a^n\, e^{-\beta a^2}\, da$$
$$= \frac{2k\beta^{(n+1)/2}}{\Gamma((n+1)/2)} \int_V a^n\, e^{-a^2(\frac{\|\mathbf{h}_s\|^\alpha}{b} + \frac{\mathbf{h}_t^\delta}{c} + \beta)}\, da$$
$$= \frac{k\beta^{(n+1)/2}}{\left(\frac{\|\mathbf{h}_s\|^\alpha}{b} + \frac{h_t^\delta}{c} + \beta\right)^{(n+1)/2}}, \tag{10}$$

where $\boldsymbol{\Theta_1} = (b, c, n, k, \alpha, \beta, \delta)$;

$$C_{s,t}(\mathbf{h}_s, h_t; \boldsymbol{\Theta_2}) = \int_V \left[k_1\, e^{-\frac{a\|\mathbf{h}_s\|^\alpha}{b}} \cdot e^{-\frac{a h_t^\delta}{c}} + k_2\, e^{-\frac{a\|\mathbf{h}_s\|^\alpha}{b}} + k_3\, e^{-\frac{a h_t^\delta}{c}} \right] \times \frac{2\beta^{(n+1)/2}}{\Gamma((n+1)/2)}\, a^n\, e^{-\beta a^2}\, da$$

$$= k_1 \frac{\beta^{(n+1)/2}}{\left(\frac{\|\mathbf{h}_s\|^\alpha}{b} + \frac{h_t^\delta}{c} + \beta\right)^{(n+1)/2}} + k_2 \frac{\beta^{(n+1)/2}}{\left(\frac{\|\mathbf{h}_s\|^\alpha}{b} + \beta\right)^{(n+1)/2}} + k_3 \frac{\beta^{(n+1)/2}}{\left(\frac{h_t^\delta}{c} + \beta\right)^{(n+1)/2}}, \tag{11}$$

where $\boldsymbol{\Theta_2} = (b, c, n, k_1, k_2, k_3, \alpha, \beta, \delta)$.

Example 3. Given the functions

$$C_s(\mathbf{h}_s; a, \omega) = \cos[a(\omega\|\mathbf{h}_s\|)], \quad a > 0,\ \omega \in \Re,$$
$$C_t(h_t; a, c, \delta) = e^{-\frac{a h_t^\delta}{c}}, \quad 1 \le \delta \le 2,\ c > 0,$$
$$\phi(a, \beta) = \beta\, e^{-a\beta}, \quad \beta > 0,$$

since the hypotheses of Theorem 1 are satisfied, two new classes of nonseparable space-time covariances are obtained:

$$C_{s,t}(\mathbf{h}_s, h_t; \boldsymbol{\Theta_1}) = \int_V k\, e^{-\frac{a h_t^\delta}{c}} \cos[a(\omega\|\mathbf{h}_s\|)] \cdot \beta\, e^{-a\beta}\, da$$
$$= k\beta \int_V e^{-a\left(\frac{h_t^\delta}{c} + \beta\right)} \cos[a(\omega\|\mathbf{h}_s\|)]\, da$$
$$= \frac{k\beta\left(\frac{h_t^\delta}{c} + \beta\right)}{\left(\frac{h_t^\delta}{c} + \beta\right)^2 + (\omega\|\mathbf{h}_s\|)^2}, \tag{12}$$

where $\boldsymbol{\Theta_1} = (c, k, \omega, \beta, \delta)$;

$$C_{s,t}(\mathbf{h}_s, h_t; \boldsymbol{\Theta_2}) = \int_V \left\{ k_1\, e^{-\frac{a h_t^\delta}{c}} \cos[a(\omega\|\mathbf{h}_s\|)] + k_2 \cos[a(\omega\|\mathbf{h}_s\|)] + k_3\, e^{-\frac{a h_t^\delta}{c}} \right\} \cdot \beta\, e^{-a\beta}\, da$$

$$= k_1 \frac{\beta\left(\frac{h_t^\delta}{c}+\beta\right)}{\left(\frac{h_t^\delta}{c}+\beta\right)^2+(\omega\|\mathbf{h}_s\|)^2} + k_2 \frac{\beta^2}{\beta^2+(\omega\|\mathbf{h}_s\|)^2} + k_3 \frac{\beta}{\frac{h_t^\delta}{c}+\beta}, \tag{13}$$

where $\boldsymbol{\Theta}_2 = (c, k_1, k_2, k_3, \omega, \beta, \delta)$.

Example 4. Given the functions

$$C_s(\mathbf{h}_s; a, \omega) = \cos[a(2\omega\|\mathbf{h}_s\|)], \quad a > 0,\ \omega \in \Re,$$
$$C_t(h_t; a, c, \delta) = e^{-\frac{a^2 h_t^\delta}{c}}, \quad 1 \le \delta \le 2,\ c > 0,$$
$$\phi(a, \beta) = \left(2\sqrt{\frac{\beta}{\pi}}\right) e^{-a^2\beta}, \quad \beta > 0,$$

since the hypotheses of Theorem 1 are satisfied, two new classes of nonseparable space-time covariances are obtained:

$$\begin{aligned} C_{s,t}(\mathbf{h}_s, h_t; \boldsymbol{\Theta}_1) &= \int_V k\ \cos[a(2\omega\|\mathbf{h}_s\|)]\, e^{-\frac{a^2 h_t^\delta}{c}} \left(2\sqrt{\frac{\beta}{\pi}}\right) e^{-a^2\beta}\, da \\ &= 2k\sqrt{\frac{\beta}{\pi}} \int_V e^{-a^2(\frac{h_t^\delta}{c}+\beta)} \cos[a(2\omega\|\mathbf{h}_s\|)]\, da \\ &= k\sqrt{\frac{\beta}{\frac{h_t^\delta}{c}+\beta}}\ e^{-\frac{\omega^2\|\mathbf{h}_s\|^2}{\frac{h_t^\delta}{c}+\beta}}, \end{aligned} \tag{14}$$

where $\boldsymbol{\Theta}_1 = (c, k, \omega, \beta, \delta)$;

$$\begin{aligned} C_{s,t}(\mathbf{h}_s, h_t; \boldsymbol{\Theta}_2) &= \int_V \left\{ k_1 \cos[a(2\omega\|\mathbf{h}_s\|)]\, e^{-\frac{a^2 h_t^\delta}{c}} + k_2 \cos[a(2\omega\|\mathbf{h}_s\|)] \right. \\ &\quad \left. + k_3\, e^{-\frac{a^2 h_t^\delta}{c}} \right\} \left(2\sqrt{\frac{\beta}{\pi}}\right) e^{-a^2\beta}\, da \\ &= k_1\sqrt{\frac{\beta}{\frac{h_t^\delta}{c}+\beta}}\ e^{-\frac{\omega^2\|\mathbf{h}_s\|^2}{\frac{h_t^\delta}{c}+\beta}} + k_2\, e^{-\frac{\omega^2\|\mathbf{h}_s\|^2}{\beta}} + k_3\sqrt{\frac{\beta}{\frac{h_t^\delta}{c}+\beta}}, \end{aligned} \tag{15}$$

where $\boldsymbol{\Theta}_2 = (c, k_1, k_2, k_3, \omega, \beta, \delta)$.

Example 5. Given the functions

$$C_s(\mathbf{h}_s; a, b, \alpha) = e^{-\frac{a^2\|\mathbf{h}_s\|^\alpha}{b}}\, e^{-\frac{\|\mathbf{h}_s\|}{a^2}}, \quad 1 \le \alpha \le 2,\ b > 0,$$
$$C_t(h_t; a, c, \delta) = e^{-\frac{a^2 h_t^\delta}{c}}\, e^{-\frac{h_t}{a^2}}, \quad 1 \le \delta \le 2,\ c > 0,$$
$$\phi(a, \beta) = 2\sqrt{\frac{\beta}{\pi}}\, e^{-a^2\beta}, \quad \beta > 0,$$

since the hypotheses of Theorem 1 are satisfied, two new classes of nonseparable space-time covariances are obtained:

$$\begin{aligned} C_{s,t}(\mathbf{h}_s, h_t; \boldsymbol{\Theta}_1) &= \int_V k\, e^{-(\frac{a^2\|\mathbf{h}_s\|^\alpha}{b} + \frac{\|\mathbf{h}_s\|}{a^2})}\ e^{-(\frac{a^2 h_t^\delta}{c} + \frac{h_t}{a^2})}\, 2\sqrt{\frac{\beta}{\pi}}\, e^{-a^2\beta}\, da \\ &= 2\sqrt{\frac{\beta}{\pi}} \int_V k\, e^{-[a^2(\beta + \frac{\|\mathbf{h}_s\|^\alpha}{b} + \frac{h_t^\delta}{c}) + \frac{\|\mathbf{h}_s\| + h_t}{a^2}]}\, da \\ &= k\sqrt{\frac{\beta}{\beta + \frac{\|\mathbf{h}_s\|^\alpha}{b} + \frac{h_t^\delta}{c}}}\ e^{-2\sqrt{(\beta + \frac{\|\mathbf{h}_s\|^\alpha}{b} + \frac{h_t^\delta}{c})(\|\mathbf{h}_s\| + h_t)}}, \end{aligned} \tag{16}$$

where $\boldsymbol{\Theta}_1 = (b, c, k, \alpha, \beta, \delta)$;

$$\begin{aligned} C_{s,t}(\mathbf{h}_s, h_t; \boldsymbol{\Theta}_2) = \int_V \Bigg[& k_1\, e^{-(\frac{a^2\|\mathbf{h}_s\|^\alpha}{b} + \frac{\|\mathbf{h}_s\|}{a^2})}\, e^{-(\frac{a^2 h_t^\delta}{c} + \frac{h_t}{a^2})} + k_2\, e^{-(\frac{a^2\|\mathbf{h}_s\|^\alpha}{b} + \frac{\|\mathbf{h}_s\|}{a^2})} \\ & + k_3\, e^{-(\frac{a^2 h_t^\delta}{c} + \frac{h_t}{a^2})} \Bigg] 2\sqrt{\frac{\beta}{\pi}}\, e^{-a^2\beta}\, da \\ = {} & k_1 \sqrt{\frac{\beta}{\beta + \frac{\|\mathbf{h}_s\|^\alpha}{b} + \frac{h_t^\delta}{c}}}\ e^{-2\sqrt{(\beta + \frac{\|\mathbf{h}_s\|^\alpha}{b} + \frac{h_t^\delta}{c})(\|\mathbf{h}_s\| + h_t)}} + k_2 \sqrt{\frac{\beta}{\beta + \frac{\|\mathbf{h}_s\|^\alpha}{b}}} \\ & \times e^{-2\sqrt{(\beta + \frac{\|\mathbf{h}_s\|^\alpha}{b})\|\mathbf{h}_s\|}} + k_3 \sqrt{\frac{\beta}{\beta + \frac{h_t^\delta}{c}}}\ e^{-2\sqrt{(\beta + \frac{h_t^\delta}{c})h_t}}, \end{aligned} \tag{17}$$

where $\boldsymbol{\Theta}_2 = (b, c, k_1, k_2, k_3, \alpha, \beta, \delta)$.

Remarks.

- Even though the space-time covariance or variogram models (since any of the above covariance models can be written in terms of variograms) look different from the spatial and temporal structures which are used in the

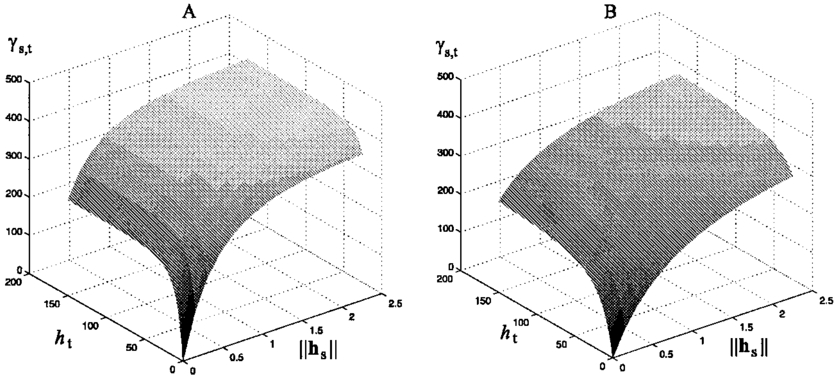

Figure 1. Integrated product–sum variogram models (9) and (11) respectively in (A) and (B), with $\boldsymbol{\Theta}_2 = (4000; 8; 2; 180; 220; 70; 1; 3; 1)$.

integrals (4)–(7), they retain the main features of the separate components in space and time;

- the integrated product–sum variogram models corresponding to (9) and (11), derived from Examples 1 and 2, with $\boldsymbol{\Theta}_2 = (4000; 8; 2; 180; 220; 70; 1; 3; 1)$, furnish a space-time variogram surface which is convex both in $\|\mathbf{h}_s\|$ and in h_t, starting from spatial and temporal exponential variogram models (Fig. 1(A) and (B));
- when the separate spatial and temporal structures are Gaussian models, the space-time variograms corresponding to (9) and (11), with $\boldsymbol{\Theta}_2 = (4000^2; 8^2; 2; 180; 220; 70; 2; 3; 2)$, turn out to be concave both in $\|\mathbf{h}_s\|$ and in h_t, especially for small spatial and temporal lags (Fig. 2(A) and (B));

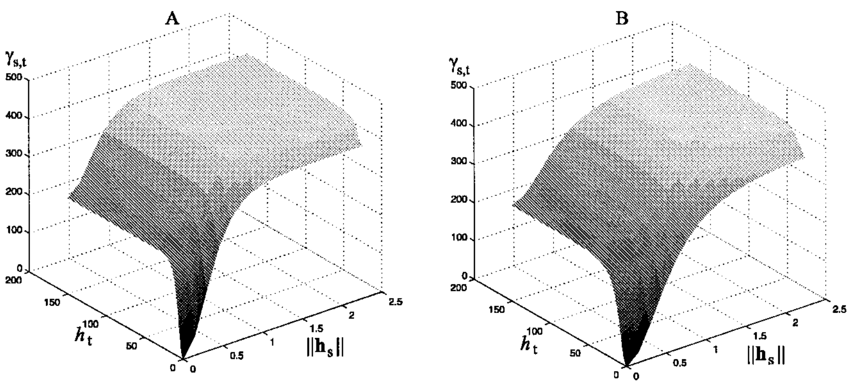

Figure 2. Integrated product–sum variogram models (9) and (11) respectively in (A) and (B), with $\boldsymbol{\Theta}_2 = (4000^2; 8^2; 2; 180; 220; 70; 2; 3; 2)$.

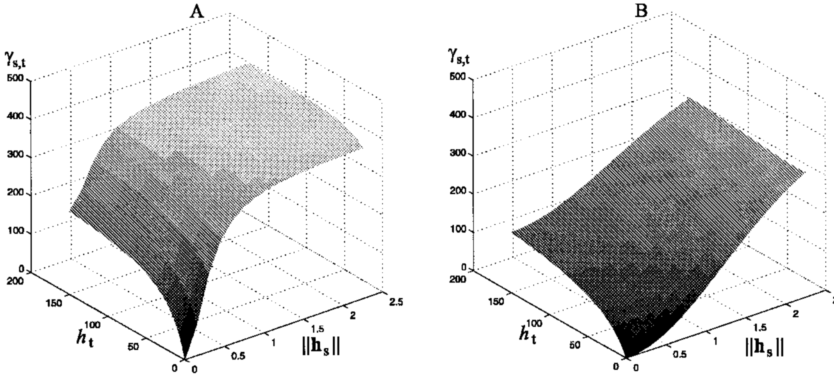

Figure 3. Integrated product–sum variogram models (13) and (15) respectively in (A) and (B), with $\mathbf{\Theta_2} = (8; 180; 220; 70; 10^{-4}; 3; 1)$.

- models (13) and (15) present parabolic behavior in $\|\mathbf{h}_s\|$ for small spatial lags; they are also either convex in h_t (Fig. 3(A) and (B)), where $\mathbf{\Theta_2} = (8; 180; 220; 70; 10^{-4}; 3; 1)$, if the temporal variogram is an exponential model, or concave in h_t (Fig. 4(A) and (B)), with $\mathbf{\Theta_2} = (8; 180; 220; 70; 10^{-4}; 3; 2)$, especially for small lags, if the temporal variogram is a Gaussian model;
- model (17), with $\mathbf{\Theta_2} = (4000^2; 8^2; 180; 220; 70; 1; 3; 1)$, can be used to describe an almost complete lack of space-time correlation, that is, it is close to a pure nugget effect model in space-time domain (Fig. 5).

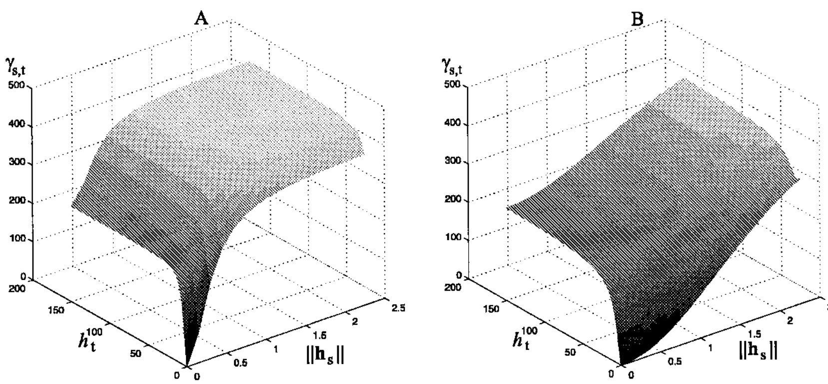

Figure 4. Integrated product–sum variogram models (13) and (15) respectively in (A) and (B), with $\mathbf{\Theta_2} = (8; 180; 220; 70; 10^{-4}; 3; 2)$.

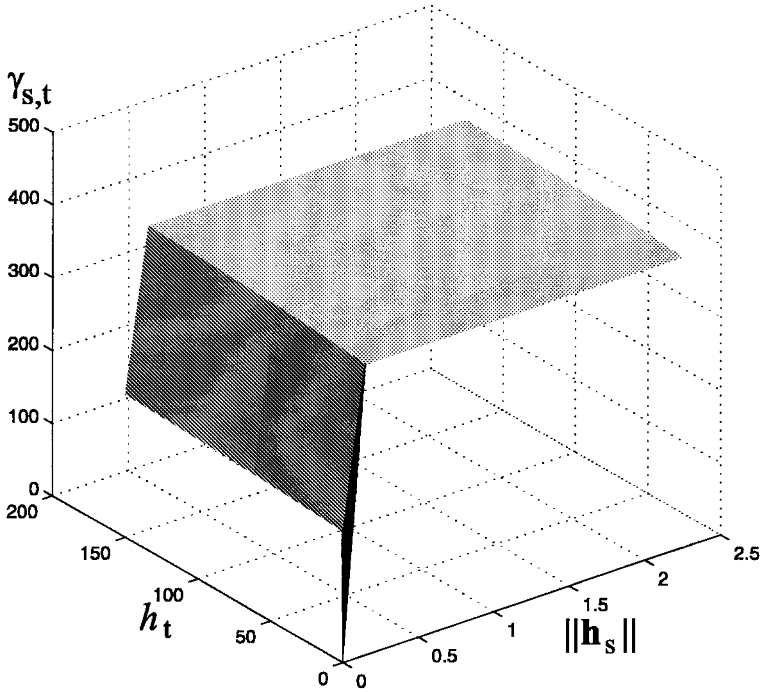

Figure 5. Integrated product–sum variogram model (17) with $\mathbf{\Theta}_2 = (4000^2; 8^2; 180; 220; 70; 1; 3; 1)$.

SOME PRACTICAL ASPECTS

Given a spatial-temporal data set, it is necessary to know how to use the data to generate a model of the form (6) or (7), that is, how to choose the function ϕ, the spatial and the temporal variograms, as well as the coefficients using the data. In the following only the practical aspects of using (7) are considered, since users can easily extend the following technique in order to utilize (6).

The first step is to take advantage of a basic property of the variogram, $\gamma(0) = 0$. Hence, from (7) it follows that

$$\gamma_{s,t}(\mathbf{h}_s, 0) = \int_V (k_2 + k_1 C_t(0; a))\, \gamma_s(\mathbf{h}_s; a)\phi(a)\, da, \tag{18}$$

and

$$\gamma_{s,t}(\mathbf{0}, h_t) = \int_V (k_3 + k_1 C_s(\mathbf{0}; a))\gamma_t(h_t; a)\phi(a)\, da. \tag{19}$$

Secondly, if it is assumed that

1. ϕ is a density function;
2. $\gamma_s(\mathbf{h}_s; a)$ and $\gamma_t(h_t; a)$ are standardized variograms with sill values equal to 1, that is, $C_s(\mathbf{0}; a) = 1$ and $C_t(0; a) = 1$; and
3. $(k_2 + k_1 C_t(0; a))C_s(\mathbf{0}; a) = (k_2 + k_1)$ and $(k_3 + k_1 C_s(\mathbf{0}; a))C_t(0; a) = (k_3 + k_1)$ are the sill values, respectively, of $\gamma_{s,t}(\mathbf{h}_s, 0)$ and $\gamma_{s,t}(\mathbf{0}, h_t)$ (De Iaco, Myers, and Posa, 2001);

then the relations between $\gamma_{s,t}(\mathbf{h}_s, 0)$ and $\gamma_s(\mathbf{h}_s; a)$, $\gamma_{s,t}(\mathbf{0}, h_t)$, and $\gamma_t(h_t; a)$ are strictly linked to the function ϕ. The above assumptions are satisfied, for example, if the parameter a is related only to the ranges of the spatial and temporal variogram models, $\gamma_s(\mathbf{h}_s; a)$ and $\gamma_t(h_t; a)$ (see examples in the previous section).

The function ϕ, which appears in the spatial-temporal variogram model in (7), can be obtained as follows:

- models for $\gamma_s(\cdot; a)$ and $\gamma_t(\cdot; a)$, dependent on a, can be chosen by looking at the behavior of the sample spatial and temporal variograms (denoted by $\hat{\gamma}_{s,t}(\mathbf{r}_s, 0)$ and $\hat{\gamma}_{s,t}(\mathbf{0}, r_t)$, respectively);
- for a discrete number of values $a_1, \ldots, a_m$ for the parameter a, one can obtain multiple spatial and temporal theoretical curves

$$\gamma_s(\cdot; a_j), \gamma_t(\cdot; a_j), \quad j = 1, \ldots, m,$$

  which provide different fits to the corresponding sample variograms $\hat{\gamma}_{s,t}(\mathbf{r}_s, 0)$ and $\hat{\gamma}_{s,t}(\mathbf{0}, r_t)$. In practice, the minimum and maximum values of the sequence $(a_i, i = 1, \ldots, m)$ are chosen in such a way that the corresponding theoretical variograms are not too "far" from the sample variograms;
- evaluate how well each $\gamma_s(\cdot; a_j)$ and $\gamma_t(\cdot; a_j)$ fits the data. This measure of the goodness of fit can be used to define a likelihood of fit and hence a probability density:

$$w_j^s = \frac{1}{\sum_{N_s} \left(\frac{\hat{\gamma}_{s,t}(\mathbf{r}_s, 0) - (k_2 + k_1)\gamma_s(\mathbf{r}_s; a_j)}{(k_2 + k_1)\gamma_s(\mathbf{r}_s; a_j)} \right)^2}, \quad j = 1, \ldots, m \tag{20}$$

$$w_j^t = \frac{1}{\sum_{N_t} \left(\frac{\hat{\gamma}_{s,t}(\mathbf{0}, r_t) - (k_3 + k_1)\gamma_t(r_t; a_j)}{(k_3 + k_1)\gamma_t(r_t; a_j)} \right)^2}, \quad j = 1, \ldots, m \tag{21}$$

  where N_s and N_t are, respectively, the number of spatial and temporal lags for the sample variograms;

- by plotting a_j versus w_j^{s} and w_j^{t}, $j = 1, \ldots, m$, one can easily define the measure ϕ;
- finally, a space-time variogram model can be obtained by solving the integral (7).

It is evident that the above model still has an unknown parameter k_1, which can be estimated in either of two ways:

- by minimizing $W(k_1)$, the weighted least-squares value (Cressie, 1993), given by

$$W(k_1) = \sum_{\mathrm{s}}^{N_{\mathrm{s}}} \sum_{\mathrm{t}}^{N_{\mathrm{t}}} |L(\mathbf{r}_{\mathrm{s}}, r_{\mathrm{t}})| \left(\frac{\hat{\gamma}_{\mathrm{s,t}}(\mathbf{r}_{\mathrm{s}}, r_{\mathrm{t}}) - \gamma_{\mathrm{s,t}}(\mathbf{r}_{\mathrm{s}}, r_{\mathrm{t}}; k_1)}{\gamma_{\mathrm{s,t}}(\mathbf{r}_{\mathrm{s}}, r_{\mathrm{t}}; k_1)} \right)^2,$$

  where $|L(\mathbf{r}_{\mathrm{s}}, r_{\mathrm{t}})|$ is the cardinality of the set

$$L(\mathbf{r}_{\mathrm{s}}, r_{\mathrm{t}}) = \{(\mathbf{s} + \mathbf{h}_{\mathrm{s}}, t + h_{\mathrm{t}}) \in A, (\mathbf{s}, t) \in A\colon \mathbf{h}_{\mathrm{s}} \in Tol(\mathbf{r}_{\mathrm{s}}) \text{ and } h_{\mathrm{t}} \in Tol(r_{\mathrm{t}})\},$$

  $Tol(\mathbf{r}_{\mathrm{s}})$, $Tol(r_{\mathrm{t}})$ are, respectively, specified tolerance regions around $\mathbf{r}_{\mathrm{s}}$ and r_{t}, N_{s} and N_{t} are, respectively, the number of spatial vector lags and the number of temporal lags, while $\hat{\gamma}_{\mathrm{s,t}}$ is the sample space-time variogram;
- by computing the sill value of $\gamma_{\mathrm{s,t}}$ from the sample space-time variogram $\hat{\gamma}_{\mathrm{s,t}}$ and solving the linear system of the following equations:

$$\begin{aligned} k_2 + k_1 &= \text{estimated sill value of } \gamma_{\mathrm{s,t}}(\mathbf{r}_{\mathrm{s}}, 0), \\ k_3 + k_1 &= \text{estimated sill value of } \gamma_{\mathrm{s,t}}(\mathbf{0}, r_{\mathrm{t}}), \\ k_1 + k_2 + k_3 &= \text{estimated sill value of } \gamma_{\mathrm{s,t}}(\mathbf{r}_{\mathrm{s}}, r_{\mathrm{t}}). \end{aligned}$$

  The method described above for generating the measure μ provides a very useful result for approximation and optimization.

Theorem 2. *Let $\phi(a)$ be a probability density function and let $\gamma_{\mathrm{s}}(\mathbf{r}_{\mathrm{s}}; a)$ and $\gamma_{\mathrm{t}}(r_{\mathrm{t}}; a)$ be standardized variograms. The spatial and temporal variograms, defined, respectively, in* (18) *and* (19), *satisfy the following inequalities:*

$$\sum_{N_{\mathrm{s}}} [\gamma_{\mathrm{s,t}}(\mathbf{r}_{\mathrm{s}}, 0) - \hat{\gamma}_{\mathrm{s,t}}(\mathbf{r}_{\mathrm{s}}, 0)]^2 \leq E_a \left(\sum_{N_{\mathrm{s}}} [\gamma_{\mathrm{s}}(\mathbf{r}_{\mathrm{s}}; a) - \hat{\gamma}_{\mathrm{s,t}}(\mathbf{r}_{\mathrm{s}}, 0)]^2 \right),$$

$$\sum_{N_{\mathrm{t}}} [\gamma_{\mathrm{s,t}}(\mathbf{0}, r_{\mathrm{t}}) - \hat{\gamma}_{\mathrm{s,t}}(\mathbf{0}, r_{\mathrm{t}})]^2 \leq E_a \left(\sum_{N_{\mathrm{t}}} [\gamma_{\mathrm{t}}(r_{\mathrm{t}}; a) - \hat{\gamma}_{\mathrm{s,t}}(\mathbf{0}, r_{\mathrm{t}})]^2 \right),$$

where $\mathbf{r}_s$ *and* r_t *have been defined in Section 2,* N_s *and* N_t *are, respectively, the number of spatial vector lags, and the number of temporal lags, and* $\hat{\gamma}_{s,t}(\mathbf{r}_s, 0)$ *and* $\hat{\gamma}_{s,t}(\mathbf{0}, r_t)$ *are the sample spatial and temporal variograms.*

Proof: Since ϕ is a density function defining

$$\gamma_{s,t}(\mathbf{r}_s, 0) = \int_0^\infty \gamma_s(\mathbf{r}_s, a)\phi(a)\, da,$$
$$\gamma_{s,t}(\mathbf{0}, r_t) = \int_0^\infty \gamma_t(r_t, a)\phi(a)\, da,$$

it follows that

$$\gamma_{s,t}(\mathbf{r}_s, 0) = E_a(\gamma_s(\mathbf{r}_s, a)),$$
$$\gamma_{s,t}(\mathbf{0}, r_t) = E_a(\gamma_t(r_t, a)).$$

Likewise,

$$\begin{aligned}
\mathrm{Var}_a(\gamma_s(\mathbf{r}_s, a)) &= E_a(\gamma_s(\mathbf{r}_s, a) - \gamma_{s,t}(\mathbf{r}_s, 0))^2 \\
&= E_a(\gamma_s(\mathbf{r}_s, a) - \hat{\gamma}_{s,t}(\mathbf{r}_s, 0))^2 - (\gamma_{s,t}(\mathbf{r}_s, 0) - \hat{\gamma}_{s,t}(\mathbf{r}_s, 0))^2, \\
\mathrm{Var}_a(\gamma_t(r_t, a)) &= E_a(\gamma_t(r_t, a) - \gamma_{s,t}(\mathbf{0}, r_t))^2 \\
&= E_a(\gamma_t(r_t, a) - \hat{\gamma}_{s,t}(\mathbf{0}, r_t))^2 - (\gamma_{s,t}(\mathbf{0}, r_t) - \hat{\gamma}_{s,t}(\mathbf{0}, r_t))^2.
\end{aligned}$$

Since the variance is nonnegative, the following inequalities hold for any lag $\mathbf{r}_s$ and r_t:

$$(\gamma_{s,t}(\mathbf{r}_s, 0) - \hat{\gamma}_{s,t}(\mathbf{r}_s, 0))^2 \le E_a(\gamma_s(\mathbf{r}_s, a) - \hat{\gamma}_{s,t}(\mathbf{r}_s, 0))^2,$$
$$(\gamma_{s,t}(\mathbf{0}, r_t) - \hat{\gamma}_{s,t}(\mathbf{0}, r_t))^2 \le E_a(\gamma_t(r_t, a) - \hat{\gamma}_{s,t}(\mathbf{0}, r_t))^2,$$

hence, the theorem follows.

This result ensures that the spatial and temporal variogram models, $\gamma_{s,t}(\mathbf{r}_s, 0)$ and $\gamma_{s,t}(\mathbf{0}, r_t)$, obtained by the above procedure, provide a better average fitting to the spatial and temporal sample variograms than the fit obtained by just using $\gamma_s(\mathbf{r}_s, \cdot)$ and $\gamma_t(r_t, \cdot)$.

AN APPLICATION TO AN AIR POLLUTION STUDY

The methods described above have been applied to hourly average concentrations of $NO_2(\mu g/m^3)$ measured during August 1997 in 18 survey stations in Milan district. After removing the seasonal component by the standard technique of moving averages (Brockwell and Davis, 1987), residuals, available for all stations, were used for the structural analysis.

The steps for generating the space-time variogram model are listed below.

- By examining the shapes of the sample spatial and temporal variograms, $\hat{\gamma}_{s,t}(\cdot, 0)$ and $\hat{\gamma}_{s,t}(\mathbf{0}, \cdot)$, the following exponential models have been chosen for $\gamma_s(\cdot, a)$ and $\gamma_t(\cdot, a)$:

$$\gamma_s(\mathbf{h}_s, a) = 1 - e^{-a\frac{\|\mathbf{h}_s\|}{4414}}, \tag{22}$$

$$\gamma_t(h_t, a) = 1 - e^{-a\frac{h_t}{8.22}}. \tag{23}$$

  The sill values have been set to 400 and 250, respectively, for the spatial and temporal structures, that is, $k_2 + k_1 = 400$ and $k_3 + k_1 = 250$. For $a = 1$, $400\gamma_s(\mathbf{h}_s, a)$ and $250\gamma_t(h_t, a)$ are considered to be a good fit to the estimated spatial and temporal variograms (Fig. 6(A) and (B)).
- After choosing 10 values of a, from $a_1 = 0.25$ to $a_{10} = 2.75$, as many spatial and temporal theoretical curves, from (22) and (23), have been obtained.

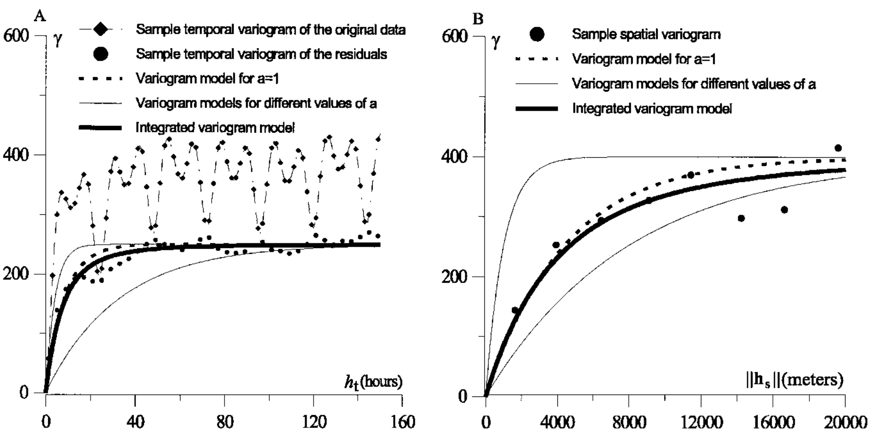

Figure 6. Sample variograms, models for different values of the parameter a, and integrated models for time (A) and space (B).

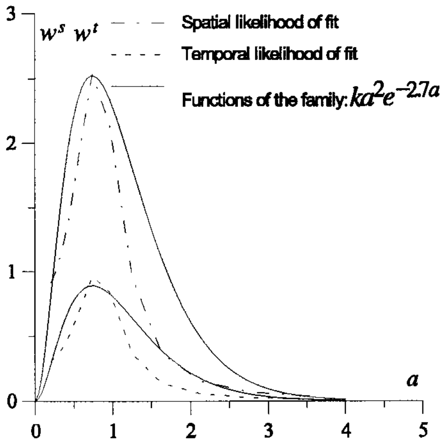

Figure 7. Spatial and temporal likelihoods of fit.

- (20) and (21) have been computed for the 10 values of a and the plot of a_j versus w_j^{s} and w_j^{t}, $j = 1, \ldots, 10$, is presented in Figure 7. Since the family of functions $ka^2\, e^{-2.7a}$ has been used for the fit, the following density function ϕ has been derived:

$$\phi(a) = 9.84a^2\, e^{-2.7a}.$$

- By using (18) and (19), the following spatial and temporal variogram models have been obtained:

$$\gamma_{\mathrm{s,t}}(\mathbf{h}_{\mathrm{s}}, 0) = \int_0^{\infty} \left[400\left(1 - e^{-a\frac{\|\mathbf{h}_{\mathrm{s}}\|}{4414}}\right)\right][9.84a^2\, e^{-2.7a}]\, da$$
$$= 400\left(1 - \frac{2.7^3}{\left(2.7 + \frac{\|\mathbf{h}_{\mathrm{s}}\|}{4414}\right)^3}\right);$$
$$\gamma_{\mathrm{s,t}}(\mathbf{0}, h_{\mathrm{t}}) = \int_0^{\infty} \left[250\left(1 - e^{-a\frac{h_{\mathrm{t}}}{8.22}}\right)\right][9.84a^2\, e^{-2.7a}]\, da$$
$$= 250\left(1 - \frac{2.7^3}{\left(2.7 + \frac{h_{\mathrm{t}}}{8.22}\right)^3}\right).$$

The sample variograms of the residuals, the exponential models for different values of a, and the integrated models are shown in Figure 6(A) and (B); moreover, the sample temporal variogram of the original data is presented (Fig. 6(A)).

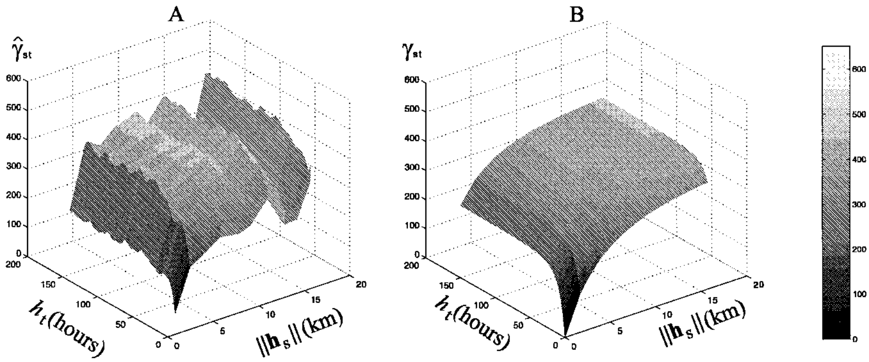

Figure 8. Sample space-time variogram surface (A) and integrated space-time variogram model (B) of residuals.

- Finally, the sill value of $\gamma_{s,t}$, evaluated from the sample space-time variogram $\hat{\gamma}_{s,t}$ (Fig. 8(A)), has been set to 470 ($k_1 + k_2 + k_3 = 470$). Hence, $k_1 = 180$, $k_2 = 220$, $k_3 = 70$ and the space-time variogram model (Fig. 8(B)) has been obtained by solving integral (7):

$$\gamma_{s,t}(\mathbf{h}_s, h_t) = 470 - 220\left(\frac{2.7}{2.7 + \frac{\|\mathbf{h}_s\|}{4414}}\right)^3 - 70\left(\frac{2.7}{2.7 + \frac{h_t}{8.2}}\right)^3$$
$$- 180\left(\frac{2.7}{2.7 + \frac{\|\mathbf{h}_s\|}{4414} + \frac{h_t}{8.22}}\right)^3.$$

CONCLUSIONS

Estimating and modeling the correlation of a space-time process is a relevant issue. In this paper, beginning with the product and the product–sum covariance models, nonintegrable space-time covariance models have been generated. These parametric families cannot be obtained, in general, from Cressie–Huang representation. To use these models, the user still must fit a model to the data. Possible choices can be determined after computing the sample spatial-temporal variogram and inspecting its main features (such as behavior near the origin for small spatial and temporal lags, the sill values along spatial and temporal directions). It is evident, for example, that one can choose between the integrated product and the integrated product–sum just by looking at the spatial and temporal sill values, since only the product–sum model can be used when the sill values are different. Several examples reproduce the most common space-time variogram behavior. Other practical aspects, linked with the problems of fitting the covariance or variogram model to the data available, were discussed and a case study has been presented.

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