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An integral transform approach to cross-variograms modeling

Salim U. Rehman, A. Shapiro *

School of Industrial and Systems Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA

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Abstract

This paper introduces cross-variograms modeling by integral transforms. The suggested models can be asymmetric and hence do not require shifting to produce asymmetric cross-variograms. These models are capable of providing anisotropic cross-variograms over multidimensional spaces. Simultaneous modeling of the cross-variograms is stressed and a method based on factorization of the unknown model coefficients is introduced. The suggested approach enables to retain joint conditional negative definiteness of the fitted models without requiring any additional constraints. Weighted least squares criterion is used to fit models to the experimental values and iterative quadratic programming is employed to solve the obtained nonlinear programming problem. Flexibility of the approach is demonstrated by fitting models to experimental cross-variograms over one-and two-dimensional spaces.

Keywords: Cross-variogram; Cokriging; Negative definiteness; Fourier transform; Hermitian matrix

1. Introduction

Fitting permissible functions to experimental variograms/cross-variograms is an essential step in cokriging. Parametric methods exist for cross-variogram fitting (Journel and Huijbregts, 1978), but such methods are restrictive as to the choice of the models for cross-variograms and may result in poor fits. In addition, these methods may become totally inapplicable in cases where different types of models need to be fitted to different variograms.

In some of the reported studies, the Cauchy–Schwartz inequality is satisfied whether using the cross-covariances or using the cross-variograms (Ahmed and De Marsity,

* Corresponding author.

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1987). It can be shown that Cauchy–Schwartz inequality is necessary but not sufficient for joint non-negative definiteness of the fitted cross-covariance models. There is a controversy over the applicability of the Cauchy–Schwartz inequality to the cross-variogram matrices (Clark et al., 1987).

In parametric set up, the requirement of joint conditional negative definiteness of the fitted functions is usually verified by checking the non-negativeness of the determinants of the corresponding coefficient matrices (Journel and Huijbregts, 1978). This puts a serious constraint over the number of variables which can be handled. This problem can be tackled by fitting the models to the variograms and cross-variograms simultaneously (Goulard and Voltz, 1992). The need of asymmetric functions for parametric modeling of cross-variograms, in principle, can be resolved by shifting the symmetric models (Journel and Huijbregts, 1978). The effect of such shifting on the requirement of joint conditional negative definiteness of the fitted functions over multidimensional spaces is yet to be understood.

Note that modeling of the cross-variograms differs from modeling of variograms in at least three aspects. First, cross-variograms are not necessarily symmetric. Second, cross-variograms are not expected to exhibit the same type of behavior as variograms, i.e., an increase in magnitude with an increase in lag. Finally, there is no requirement of their conditional negative definiteness. In this paper, we discuss an approach to cross-variograms modeling which is suited to deal with the above-mentioned differences. This method is an extension of an approach introduced in Shapiro and Botha (1991). The suggested models can be used for any number of variables over one-, two- and three-dimensional spaces.

In Section 2 of this paper, we present a theoretical formulation of cross-variogram models and argue that valid cross-variograms should be jointly conditionally negative definite. In Section 2.1, we introduce asymmetric models for cross-variograms over a one-dimensional space. Anisotropic models over two- and three-dimensional spaces are introduced in Section 2.2.1. Isotropic and symmetric models for the same regions of support are introduced in Section 2.2.2, while anisotropic and symmetric models are covered in Section 2.2.3. Section 2.3 describes a method of acquiring asymmetry through shifting of the symmetric cross-variograms; it shows that in such cases, the shift vectors appear in the non-negative definite matrices needed to satisfy the requirement of joint conditional negative definiteness of the models. There is an opinion that fitting models to the experimental data using a criterion like least squares estimation deprives the users of any control over the fitted models and that the shape of the fit is determined by the experimental values. In Section 2.4, we describe how the user can still control the shape of the fitted models. In particular, we introduce in that section formulation of constraints enforcing smoothness, monotonicity and concavity of the fitted functions. Section 3 discusses a methodology for acquiring fit to the experimental data over one-dimensional spaces.

We demonstrate applicability of the developed procedure with the help of two examples. The first example is for one-dimensional spaces while the second one is for the case of two- dimensional spaces. The experimental cross-variograms for both examples were estimated from data observed over a two- dimensional space. In Section 4, the effects of various parameters concerning the criterion of fitting the models are discussed and some guidelines as to how these parameters can be chosen are included. Finally, in Section 5 we present concluding observations.

2. Theoretical background

We begin with some basic definitions and describe a theoretical background required for our approach to cross-variograms modeling. Consider a multivariate spatial process $\boldsymbol{Z}(\boldsymbol{s}) \equiv (Z_1(\boldsymbol{s}), ..., Z_k(\boldsymbol{s}))$, $\boldsymbol{s} \in D$, where D is a domain in $\mathbb{R}^d$. We assume subsequently that the process $\boldsymbol{Z}(\boldsymbol{s})$ is second-order stationary. The cross-variograms [1] of $\boldsymbol{Z}(\boldsymbol{s})$ are then defined as (see Cressie, 1991, Section 3.2.3)

$$2\gamma_{jj'}(\boldsymbol{h}) = \text{var}\{Z_j(\boldsymbol{s}+\boldsymbol{h}) - Z_{j'}(\boldsymbol{s})\}, \quad j,j' = 1,...,k. \tag{2.1}$$

Half of the cross-variograms, i.e., the functions $\gamma_{jj'}(\cdot)$, are called cross-semivariograms. For $j = 1,...,k$, the function $2\gamma_{jj}(\cdot)$ (the function $\gamma_{jj}(\cdot)$) is called the variogram (semivariogram) of the corresponding process $Z_j(\cdot)$. General conditions for existence of the semivariograms, $\gamma_{jj}(\cdot)$, are known as the Intrinsic Hypothesis and are discussed at length in Matheron (1963, 1971, 1973). Since in this article we model cross-variograms over a bounded domain D, the second-order stationarity assumption will suffice for our purposes.

Given n observations of a second-order stationary process, $\boldsymbol{Z}(\boldsymbol{s})$, at locations $\boldsymbol{s}_1, ..., \boldsymbol{s}_n$, a linear predictor of, say, $Z_1(\boldsymbol{s}_0)$ at a new location $\boldsymbol{s}_0$ is

$$\hat{Z}_1(\boldsymbol{s}_0) = \sum_{i=1}^{n}\sum_{j=1}^{k} \lambda_{ji} Z_j(\boldsymbol{s}_i). \tag{2.2}$$

The Best Linear Unbiased Predictor (BLUP) is then obtained by minimizing

$$\text{var}\left\{Z_1(\boldsymbol{s}_0) - \sum_{i=1}^{n}\sum_{j=1}^{k} \lambda_{ji} Z_j(\boldsymbol{s}_i)\right\}, \tag{2.3}$$

subject to the unbiasedness conditions

$$\sum_{i=1}^{n} \lambda_{1i} = 1 \quad \text{and} \quad \sum_{i=1}^{n} \lambda_{ji} = 0, \ j = 2,...,k. \tag{2.4}$$

This estimation procedure (called cokriging in Geostatistics, (Cressie, 1991, Section 3.2.3)) can be formulated in terms of the cross-semivariograms $\gamma_{jj'}(\cdot)$. For the sake of simplicity let us take $k = 2$. Then cokriging is performed by minimization

[1] Some authors use the term pseudo cross-variograms.

of

$$-\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_{1i}\lambda_{1j}\gamma_{11}(\boldsymbol{s}_i-\boldsymbol{s}_j)+2\sum_{i=1}^{n}\lambda_{1i}\gamma_{11}(\boldsymbol{s}_0-\boldsymbol{s}_i)$$

$$-2\sum_{i=1}^{n}\sum_{k=1}^{n}\lambda_{1i}\lambda_{2k}\gamma_{12}(\boldsymbol{s}_i-\boldsymbol{s}_k)+2\sum_{k=1}^{n}\lambda_{2k}\gamma_{12}(\boldsymbol{s}_0-\boldsymbol{s}_k)$$

$$-\sum_{k=1}^{n}\sum_{\ell=1}^{n}\lambda_{2k}\lambda_{2\ell}\gamma_{22}(\boldsymbol{s}_k-\boldsymbol{s}_\ell) \tag{2.5}$$

over $\lambda_{11},...,\lambda_{1n},\lambda_{21},...,\lambda_{2n}$, subject to the constraints (2.4). This optimization problem is a quadratic programming problem subject to linear equality constraints. It has an optimal solution if and only if the objective function is convex over the affine space defined by Eqs. (2.4). Since the objective function is quadratic, this is equivalent to the condition that the quadratic function

$$Q(\boldsymbol{\lambda}_1,\boldsymbol{\lambda}_2)=-\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_{1i}\lambda_{1j}\gamma_{11}(\boldsymbol{s}_i-\boldsymbol{s}_j)$$

$$-2\sum_{i=1}^{n}\sum_{k=1}^{n}\lambda_{1i}\lambda_{2k}\gamma_{12}(\boldsymbol{s}_i-\boldsymbol{s}_k)$$

$$-\sum_{k=1}^{n}\sum_{\ell=1}^{n}\lambda_{2k}\lambda_{2\ell}\gamma_{22}(\boldsymbol{s}_k-\boldsymbol{s}_\ell) \tag{2.6}$$

is non-negative definite over the linear space corresponding to the affine space defined by Eqs. (2.4). That is, $Q(\boldsymbol{\lambda}_1,\boldsymbol{\lambda}_2)\geq 0$ for any $\boldsymbol{\lambda}_1=(\lambda_{11},...,\lambda_{1n})$ and $\boldsymbol{\lambda}_2=(\lambda_{21},...,\lambda_{2n})$ satisfying

$$\sum_{i=1}^{n}\lambda_{ji}=0,\quad j=1,\ldots,k. \tag{2.7}$$

Therefore not all functions $2\gamma_{jj'}(\cdot)$ can be meaningful cross-variograms. In particular, the above condition of non-negative definiteness is important. Without that condition the corresponding optimization problem can be meaningless in the sense that it may not possess an optimal solution and the associated variance estimates can be negative. The above discussion motivates us to introduce the following definition of *permissible* (valid) cross-variograms (cross-semivariograms).

Definition 2.1. We say that a collection of functions $g_{jj'}(\cdot)$, $j,j'=1,...,k$, forms permissible cross-variograms if:

(i) These functions are continuous, except possibly at the origin.

(ii) $g_{jj'}(\boldsymbol{h})\geq 0$, $j,j'=1,...,k$, for all $\boldsymbol{h}\in\mathbb{R}^d$.

(iii) $g_{jj'}(\boldsymbol{h})=g_{j'j}(-\boldsymbol{h})$, $j,j'=1,...,k$, for all $\boldsymbol{h}\in\mathbb{R}^d$.

(iv) The functions $-g_{jj'}(\cdot)$, $j,j' = 1,\dots,k$, are conditionally non-negative definite in the sense that

$$-\sum_{\ell=1}^{n}\sum_{\ell'=1}^{n}\sum_{j=1}^{k}\sum_{j'=1}^{k} x_{j\ell}x_{j'\ell'}g_{jj'}(\boldsymbol{s}_\ell - \boldsymbol{s}_{\ell'}) \geq 0, \tag{2.8}$$

for any $\boldsymbol{s}_1,\dots,\boldsymbol{s}_n \in \mathbb{R}^d$ and any numbers $x_{j\ell}$ satisfying the equations

$$\sum_{\ell=1}^{n} x_{j\ell} = 0, \quad j = 1,\dots,k. \tag{2.9}$$

Let us make the following observations. Conditions (i)–(iv) of the above definition imply that the functions $g_{jj}(\cdot)$, $j = 1,\dots,k$, individually, are permissible variograms in the usual sense used in Geostatistics (cf. Armstrong and Diamond, 1984; Christakos, 1984; Cressie, 1991, Section 2.5.2). In particular, it follows from condition (iii) that these functions are symmetric, i.e., $g_{jj}(\boldsymbol{h}) = g_{jj}(-\boldsymbol{h})$, and it follows from condition (iv) that $-g_{jj}(\cdot)$, $j = 1,\dots,k$, are conditionally non-negative definite. Note that this symmetry does not necessarily hold for the functions $g_{jj'}(\cdot)$ when $j \neq j'$.

It is not difficult to see that if functions $f_{jj'}(\cdot), j,j' = 1,\dots,k$, are jointly non-negative definite in the sense that

$$\sum_{\ell=1}^{n}\sum_{\ell'=1}^{n}\sum_{j=1}^{k}\sum_{j'=1}^{k} x_{j\ell}x_{j'\ell'}f_{jj'}(\boldsymbol{s}_\ell - \boldsymbol{s}_{\ell'}) \geq 0, \tag{2.10}$$

for any $\boldsymbol{s}_1,\dots,\boldsymbol{s}_n \in \mathbb{R}^d$ and any numbers $x_{j\ell}$, $j = 1,\dots,k; \ell = 1,\dots,n$, then the functions $-g_{jj'}(\cdot) = f_{jj'}(\cdot) - c_{jj'}$ are jointly conditionally non-negative definite for any choice of constants $c_{jj'}$. Consequently such functions $g_{jj'}(\cdot)$ can be used to construct permissible cross-variograms.

Now, in order to generate non-negative definite functions $f_{jj'}(\cdot)$, we use the following result which is a natural generalization of the "sufficient" part of Bochner's theorem (Armstrong and Diamond, 1984). Consider the Fourier transform

$$\boldsymbol{f}(\boldsymbol{s}) = \int_{\mathbb{R}^d} e^{i\boldsymbol{s}\cdot\boldsymbol{t}} d\boldsymbol{M}(\boldsymbol{t}), \tag{2.11}$$

of a matrix valued measure $\boldsymbol{M}(\boldsymbol{t})$, $\boldsymbol{t} \in \mathbb{R}^d$. That is, $\boldsymbol{M}(\boldsymbol{t}) = [\mu_{jj'}(\boldsymbol{t})], j,\ j' = 1,\dots,k$, where $\mu_{jj'}(\cdot)$ are complex valued. Note that $\boldsymbol{f}(\boldsymbol{s}) = [f_{jj'}(\boldsymbol{s})], j,\ j' = 1,\dots,k$, where

$$f_{jj'}(\boldsymbol{s}) = \int_{\mathbb{R}^d} e^{i\boldsymbol{s}\cdot\boldsymbol{t}} d\mu_{jj'}(\boldsymbol{t}). \tag{2.12}$$

Let us show that if the measure $\boldsymbol{M}(\boldsymbol{t})$ is Hermitian non-negative definite matrix valued, then the functions $f_{jj'}(\cdot)$ are jointly non-negative definite. (Recall that a complex valued matrix $\mathscr{V} = [v_{ij}]$, $i,j = 1,\dots,n$, is called Hermitian if $v_{ji} = \bar{v}_{ij}$ and it is called non-negative definite if $\sum_{i=1}^{n}\sum_{j=1}^{n} x_i\bar{x}_j v_{ij} \geq 0$ for any complex numbers

$x_1,...,x_n$.) It will be sufficient to show this for atomic (discrete) measures. That is, let

$$f(s) = \sum_{\ell=1}^{m} e^{i s \cdot t_\ell} \mathscr{V}^\ell, \tag{2.13}$$

where $\mathscr{V}^\ell = [v^\ell_{jj'}]$, $\ell = 1,...,m$, are Hermitian non-negative definite matrices. (The matrices $\mathscr{V}^\ell$ will be called the coefficient matrices.) We have then

$$\sum_{p=1}^{n}\sum_{p'=1}^{n}\sum_{j=1}^{k}\sum_{j'=1}^{k} x_{jp}\bar{x}_{j'p'} f_{jj'}(s_p - s_{p'})$$

$$= \sum_{p=1}^{n}\sum_{p'=1}^{n}\sum_{j=1}^{k}\sum_{j'=1}^{k}\sum_{\ell=1}^{m} x_{jp}\bar{x}_{j'p'} (e^{i s_p \cdot t_\ell})(e^{-i s_{p'} \cdot t_\ell}) v^\ell_{jj'}$$

$$= \sum_{\ell=1}^{m}\sum_{j=1}^{k}\sum_{j'=1}^{k} z^\ell_j \bar{z}^\ell_{j'} v^\ell_{jj'} , \tag{2.14}$$

where $z^\ell_j = \sum_{p=1}^{n} x_{jp} e^{i s_p \cdot t_\ell}$. Since the matrices $\mathscr{V}^\ell$ are non-negative definite, we have

$$\sum_{j=1}^{k}\sum_{j'=1}^{k} z^\ell_j \bar{z}^\ell_{j'} v^\ell_{jj'} \geq 0$$

and hence the sum in (2.14) is non-negative.

Therefore we can generate a collection of jointly non-negative definite functions in the form

$$f_{jj'}(s) = \sum_{\ell=1}^{m} e^{i s \cdot t_\ell} v^\ell_{jj'} , \quad j,j' = 1,...,k, \tag{2.15}$$

where $[v^\ell_{jj'}]$, $\ell = 1,...,m$, are Hermitian non-negative definite matrices and $t_1,...,t_m$ are corresponding points in $\mathbb{R}^d$. It follows then that $f_{j'j}(-s) = \overline{f_{jj'}(s)}$. The complex numbers $v^\ell_{jj'} = a^\ell_{jj'} + ib^\ell_{jj'}$ should be chosen in such a way that the corresponding functions $f_{jj'}(\cdot)$ are real valued. The functions $g_{jj'}(\cdot) = c_{jj'} - f_{jj'}(\cdot)$, $j,j' = 1,...,k$, will then form permissible cross-variograms provided these functions are non-negative valued.

2.1. Cross-variograms over one-dimensional spaces

Let us now consider the case of $d = 1$, i.e. $s,t \in \mathbb{R}$. Since the functions $f_{jj}(s)$, $j = 1,...,k$, should be symmetric, we can write

$$f_{jj}(s) = \sum_{\ell=1}^{m} a^\ell_{jj} \cos(st_\ell) , \quad j = 1,...,k, \tag{2.16}$$

and for $1 \leq j \neq j' \leq k$, we have asymmetric functions

$$f_{jj'}(s) = \sum_{\ell=1}^{m} a_{jj'}^{\ell} \cos(st_\ell) - b_{jj'}^{\ell} \sin(st_\ell). \tag{2.17}$$

Here, $t_\ell > 0$, $\ell = 1,...,m$, and the matrices $\mathscr{V}^\ell = [v_{jj'}^\ell]$, where $v_{jj'}^\ell = a_{jj'}^\ell + ib_{jj'}^\ell$, $j,j' = 1,...,k$, should be Hermitian and non-negative definite. (Note that since $\mathscr{V}^\ell$ are Hermitian, it follows that $v_{j'j}^\ell = \bar{v}_{jj'}^\ell = a_{jj'}^\ell - ib_{jj'}^\ell$, and hence $b_{jj}^\ell = 0$, $j = 1,...,k$.) Thus the matrices $\mathscr{V}^\ell$ are given by

$$\mathscr{V}^\ell = \begin{bmatrix} a_{11}^\ell & a_{12}^\ell + ib_{12}^\ell & \cdots & a_{1k}^\ell + ib_{1k}^\ell \\ a_{12}^\ell - ib_{12}^\ell & a_{22}^\ell & \cdots & a_{2k}^\ell + ib_{2k}^\ell \\ \vdots & & \ddots & \vdots \\ a_{1k}^\ell - ib_{1k}^\ell & a_{2k}^\ell - ib_{2k}^\ell & \cdots & a_{kk}^\ell \end{bmatrix}, \quad \ell = 1,\ldots,m. \tag{2.18}$$

Now, given that $f_{jj'}(\cdot)$ are generated according to (2.16) and (2.17) and the non-negative definiteness condition holds, the functions $g_{jj'}(\cdot) = c_{jj'} - f_{jj'}(\cdot)$ are permissible cross-variograms provided these functions are non-negative valued. Note that the functions $g_{jj}(\cdot)$ are non-negative valued if and only if

$$c_{jj} - \sum_{\ell=1}^{m} a_{jj}^\ell \geq 0, \quad j = 1,...,k, \tag{2.19}$$

and a sufficient condition for non-negativeness of $g_{jj'}(\cdot)$ for $j \neq j'$ is

$$c_{jj'} - \sum_{\ell=1}^{m} \sqrt{(a_{jj'}^\ell)^2 + (b_{jj'}^\ell)^2} \geq 0. \tag{2.20}$$

For $k = 2$, the non-negative definiteness condition is equivalent to the following conditions:

$$a_{11}^\ell \geq 0, \; a_{22}^\ell \geq 0, \; \text{and} \; a_{11}^\ell a_{22}^\ell \geq (a_{12}^\ell)^2 + (b_{12}^\ell)^2, \quad \ell = 1,...,m. \tag{2.21}$$

It can immediately be seen that a_{12}^ℓ and/or b_{12}^ℓ will be non-zero only if a_{11}^ℓ and a_{22}^ℓ are both non-zero. It was experienced during cross-variograms modeling that some of the numbers a_{11}^ℓ and a_{22}^ℓ, $\ell = 1,\ldots,m$, tend to be zero. The corresponding a_{12}^ℓ and b_{12}^ℓ are then forced to be zero resulting in a poor fit of cross-variograms. This problem can be resolved by simultaneously fitting the variograms/cross-variograms.

2.1.1. Extension to more than two variables

While the simultaneous modeling technique works well for two variables, its extension to more than two variables becomes restrictive since the condition of non-negative definiteness of the coefficient matrices (2.18) is harder to satisfy using the determinant approach. A parameterization of the unknown coefficients $a_{jj'}^\ell$ and $b_{jj'}^\ell$ is one possible solution to the problem. Consider Cholesky decomposition of the coefficient matrices $\mathscr{V}^\ell = U^\ell \overline{U^\ell}$, where $U^\ell, \ell = 1,\dots,m$, are upper triangular matrices of unknowns u^ℓ_ξ and $v^\ell_\xi, \xi = 1,\dots,(k^2+k)/2$, with

$$U^\ell = \begin{bmatrix} u_1^\ell + iv_1^\ell & u_2^\ell + iv_2^\ell & \dots & u_k^\ell + iv_k^\ell \\ 0 & u_{k+1}^\ell + iv_{k+1}^\ell & \dots & u_{2k-1}^\ell + iv_{2k-1}^\ell \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & u^\ell_{(k^2+k)/2} + iv^\ell_{(k^2+k)/2} \end{bmatrix}, \quad \ell = 1,\dots,m. \tag{2.22}$$

The elements of the coefficient matrices $\mathscr{V}^\ell$ can be found to be

$$\begin{aligned} a^\ell_{jj} &= \sum_{i'=1}^{k-j+1} (u^\ell_{p_{jj}+i'})^2 + (v^\ell_{p_{jj}+i'})^2, \quad j = 1,\dots,k, \\ a^\ell_{jj'} &= \sum_{i'=1}^{k-j'+1} (u^\ell_{p_j+i'} u^\ell_{p'_j+i'} + v^\ell_{p_j+i'} v^\ell_{p'_j+i'}), \quad j < j' \le k, \\ b^\ell_{jj'} &= \sum_{i'=1}^{k-j'+1} (u^\ell_{p'_j+i'} v^\ell_{p_j+i'} - u^\ell_{p_j+i'} v^\ell_{p'_j+i'}), \quad j < j' \le k, \end{aligned} \tag{2.23}$$

where $p_{jj} = \sum_{i'=1}^{j-1}(k-i'+1)$, $p_j = j'-j+\sum_{i'=1}^{j-1}(k-i'+1)$ and $p_{j'} = \sum_{i'=1}^{j'-1}(k-i'+1)$.

The unknowns $a^\ell_{jj'}$ and $b^\ell_{jj'}$ in (2.16) and (2.17) can be replaced by the corresponding sequences of unknowns u^ℓ_ξ and v^ℓ_ξ from (2.23). The problem thus reduces to estimation of the vectors $\boldsymbol{c}$, $\boldsymbol{u}$ and $\boldsymbol{v}$ of unknowns subject to the non-negativity constraints. For $k = 2$, the permissible models can be written in the form

$$\begin{aligned} g_{11}(h) &= c_{11} - \sum_{\ell=1}^{m} [(u_1^\ell)^2 + (u_2^\ell)^2 + (v_1^\ell)^2 + (v_2^\ell)^2] \cos(ht_\ell), \\ g_{22}(h) &= c_{22} - \sum_{\ell=1}^{m} [(u_3^\ell)^2 + (v_3^\ell)^2] \cos(ht_\ell), \\ g_{12}(h) &= c_{12} - \sum_{\ell=1}^{m} \{[u_2^\ell u_3^\ell + v_2^\ell v_3^\ell] \cos(ht_\ell) - [v_2^\ell u_3^\ell - v_3^\ell u_2^\ell] \sin(ht_\ell)\}. \end{aligned} \tag{2.24}$$

The corresponding non-negativity constraints are

$$\begin{aligned} & c_{11} - \sum_{\ell=1}^{m} (u_1^\ell)^2 + (u_2^\ell)^2 + (v_1^\ell)^2 + (v_2^\ell)^2 \ge 0, \\ & c_{22} - \sum_{\ell=1}^{m} (u_3^\ell)^2 + (v_3^\ell)^2 \ge 0, \\ & c_{12} - \sum_{\ell=1}^{m} \sqrt{(u_2^\ell u_3^\ell + v_2^\ell v_3^\ell)^2 + (v_2^\ell u_3^\ell - v_3^\ell u_2^\ell)^2} \ge 0. \end{aligned} \tag{2.25}$$

2.2. Cross-variograms over multidimensional spaces

2.2.1. Asymmetric cross-variograms

An extension of the proposed method to the case of $d \geq 2$ is straightforward. For $d = 2$, with $\boldsymbol{h} = (x, y)'$, the following function can be used for modeling the cross-variograms:

$$g_{jj'}(\boldsymbol{h}) = c_{jj'} - \sum_{\ell=-m_1}^{m_1} \sum_{\ell'=-m_2}^{m_2} \mathrm{e}^{\mathrm{i}(xt_\ell + yt_{\ell'})} v_{jj'}^{\ell\ell'}. \tag{2.26}$$

The function which can be used for $d = 3$ with $\boldsymbol{h} = (x, y, z)'$ is

$$g_{jj'}(\boldsymbol{h}) = c_{jj'} - \sum_{\ell=-m_1}^{m_1} \sum_{\ell'=-m_2}^{m_2} \sum_{\ell''=-m_3}^{m_3} \mathrm{e}^{\mathrm{i}(xt_\ell + yt_{\ell'} + zt_{\ell''})} v_{jj'}^{\ell\ell'\ell''}. \tag{2.27}$$

The coefficient matrices $\mathscr{V}^{\ell\ell'\ell''} = [v_{jj'}^{\ell\ell'\ell''}]$ can be found by using the relations (2.18) and (2.23) after replacing the superscript ℓ with $\ell\ell'$ for $d = 2$ and with $\ell\ell'\ell''$ for $d = 3$. This formulation not only permits asymmetry of the cross-variograms but also allows anisotropies of the variograms and cross-variograms. The number of unknowns, however, increases exponentially with d and so does the CPU time during the model fitting stage.

2.2.2. Symmetric and isotropic cross-variograms

In the case of $d \geq 2$, there is a natural concept of *isotropic* variograms $g(\boldsymbol{h})$, when $g(\boldsymbol{h})$ depends on $\boldsymbol{h}$ only through its Euclidean norm $h = \|\boldsymbol{h}\|$. This, automatically, makes such functions symmetric. These functions can be useful in modeling cross-variograms when the experimental data is indicative of symmetry. In this approach, formula (2.16) can be used to construct analogues of isotropic cross-variograms by replacing $\cos(\cdot)$ functions with Bessel functions of the first kind (Shapiro and Botha, 1991). The resulting symmetric models known as Hankel transforms are functions of a single variable. The isotropic models for the cross-variograms over a two-dimensional space can be written as

$$g_{jj'}(\boldsymbol{h}) = c_{jj'} - \sum_{\ell=1}^{m} J_0(h\, t_\ell) a_{jj'}^{\ell}, \quad j, j' = 1, \ldots, k. \tag{2.28}$$

For $d = 3$, the cross-variograms can be modeled using

$$g_{jj'}(\boldsymbol{h}) = c_{jj'} - \sum_{\ell=1}^{m} \frac{\sin(h\, t_\ell)}{h t_\ell} a_{jj'}^{\ell}, \quad j, j' = 1, \ldots, k. \tag{2.29}$$

Non-negativity of these functions can be ensured by requiring

$$c_{jj'} - \sum_{\ell=1}^{m} | a_{jj'}^{\ell} | \geq 0, \quad j, j' = 1, \ldots, k. \tag{2.30}$$

Models (2.28) and (2.29) will be permissible cross-variograms if the $k \times k$ coefficient matrices $\mathscr{V}^{\ell}$ are real, symmetric and non-negative definite. This requirement can once again be met by using Cholesky decomposition of the unknown coefficients. The real and symmetric coefficient matrices $\mathscr{V}^{\ell}$ can be written as

$$\mathscr{V}^{\ell} = \begin{bmatrix} a^{\ell}_{11} & a^{\ell}_{12} & \cdots & a^{\ell}_{1k} \\ a^{\ell}_{12} & a^{\ell}_{22} & \cdots & a^{\ell}_{2k} \\ \vdots & & \ddots & \vdots \\ a^{\ell}_{1k} & a^{\ell}_{2k} & \cdots & a^{\ell}_{kk} \end{bmatrix}, \quad \ell = 1,\dots,m, \tag{2.31}$$

with their elements given by

$$\begin{aligned} a^{\ell}_{jj} &= \sum_{i'=1}^{k-j+1} (u^{\ell}_{p_{jj}+i'})^2, \quad j = 1,\dots,k, \\ a^{\ell}_{jj'} &= \sum_{i'=1}^{k-j'+1} (u^{\ell}_{p_j+i'} u^{\ell}_{p'_j+i'}), \quad j < j' \le k, \end{aligned} \tag{2.32}$$

where $p_{jj} = \sum_{i'=1}^{j-1}(k-i'+1)$, $p_j = j'-j+\sum_{i'=1}^{j-1}(k-i'+1)$ and $p_{j'} = \sum_{i'=1}^{j'-1}(k-i'+1)$.

2.2.3. Symmetric and anisotropic cross-variograms

Models (2.28) and (2.29) can easily be corrected for anisotropies. Consider transforming the lag vectors, $\boldsymbol{h}$, through multiplication with a transformation matrix $\boldsymbol{L}'$, where $\boldsymbol{L}$ is a lower triangular matrix of an appropriate size. The norm of the transformed lag vector is $\sqrt{\boldsymbol{h}'\boldsymbol{L}\boldsymbol{L}'\boldsymbol{h}}$ and the resulting anisotropic models are

$$g_{jj'}(\boldsymbol{h}) = c_{jj'} - \sum_{\ell=1}^{m} J_0([\boldsymbol{h}'\boldsymbol{L}\boldsymbol{L}'\boldsymbol{h}]^{\frac{1}{2}}\, t_\ell) a^{\ell}_{jj'} \quad \text{for } d = 2, \tag{2.33a}$$

$$g_{jj'}(\boldsymbol{h}) = c_{jj'} - \sum_{\ell=1}^{m} \frac{\sin([\boldsymbol{h}'\boldsymbol{L}\boldsymbol{L}'\boldsymbol{h}]^{1/2}\, t_\ell)}{[\boldsymbol{h}'\boldsymbol{L}\boldsymbol{L}'\boldsymbol{h}]^{1/2}\, t_\ell} a^{\ell}_{jj'} \quad \text{for } d = 3. \tag{2.33b}$$

The elements of the lower triangular matrix $\boldsymbol{L}$ can also be treated as unknowns and found during the model fitting stage. Use of identity matrices of appropriate sizes for $d = 2$ and $d = 3$ in place of $\boldsymbol{L}$ will result in isotropic cross-variograms given by (2.28) and (2.29).

2.3. Shifted cross-variograms

Asymmetric cross-variograms can also be constructed by introducing shift vectors in the arguments of the symmetric models (Journel and Huijbregts, 1978). Suppose we have symmetric one-dimensional models

$$g_{jj'}(h) = c_{jj'} - \sum_{\ell=1}^{m} \Omega^{\ell}_{jj'} \cos(h\, t_\ell), \quad j,j' = 1,\dots,k. \tag{2.34}$$

Shift arguments $\tilde{h}_{jj'}$ with $\tilde{h}_{jj} = 0$ can be introduced in these models to yield asymmetric cross-variograms

$$g_{jj'}(h) = c_{jj'} - \sum_{\ell=1}^{m} \Omega^{\ell}_{jj'} \cos(\{h + \tilde{h}_{jj'}\}\, t_\ell), \quad j, j' = 1, \ldots, k. \tag{2.35}$$

For $j \neq j'$, these models can be shown to be equivalent to the models (2.17) for $a^{\ell}_{jj'} = \Omega^{\ell}_{jj'}\cos(\tilde{h}_{jj'} t_\ell)$ and $b^{\ell}_{jj'} = \Omega^{\ell}_{jj'}\sin(\tilde{h}_{jj'} t_\ell)$. Since non-negative definiteness of the Hermitian matrices $[v^{\ell}_{jj'}], \ell = 1, \ldots, m$, with $v^{\ell}_{jj'} = a^{\ell}_{jj'} + ib^{\ell}_{jj'}$, implies joint conditional non-negative definiteness of the functions (2.16) and (2.17), we note that the matrices $[\Omega^{\ell}_{jj'} e^{i\tilde{h}_{jj'} t_\ell}]$ and not the matrices $[\Omega^{\ell}_{jj'}]$ are required to be non-negative definite. Similar expressions, involving shift vectors $\tilde{\boldsymbol{h}}_{jj'}$, can be obtained for models over multidimensional spaces.

2.4. Smoothness, monotonicity and concavity conditions

The fitted cross-variograms could follow the estimated values too closely and, especially when the estimated values are scattered, may change rapidly. In order to eliminate such noisy behavior, further constraints may be required. Smoothness, monotonicity or concavity of the fitted cross-variograms can be enforced by the corresponding constraints on their derivatives. For example, the monotonicity of $g_{jj'}(\cdot)$, in positive and negative directions, can be enforced by the constraints $g'_{jj'}(s) \geq 0$ for $s \geq 0$ and $g'_{jj'}(s) \leq 0$ for $s \leq 0$. Smoothness of $g_{jj'}(\cdot)$ can be controlled by a bound on its second-order derivatives. Likewise concavity can be acquired by restricting the choice of $g_{jj'}(s)$ to the class of functions with the property $g''_{jj'}(s) \leq 0$ for $s \geq 0$ and $g''_{jj'}(s) \geq 0$ for $s \leq 0$. Although the derivatives of the models can be used to formulate constraints as stated above, we found it convenient to use the differences. That is, for monotonicity for instance, we required $g_{jj'}(s + h) - g_{jj'}(s) \geq 0$ for $s, h > 0$.

3. Methodology and experimental results

We now discuss a methodology of fitting permissible cross-variograms to empirical data over one-dimensional spaces, i.e. for $d = 1$. Let $\hat{\gamma}_{jj'}(h)$, $j, j' = 1, \ldots, k$, be empirical cross-semivariograms estimated at lags h_i, $i = 1, \ldots, n$. For example, given observations of the process $\boldsymbol{Z}(s)$, we can use the classical estimator

$$2\hat{\gamma}_{jj'}(h) = N(h)^{-1} \sum_{\ell=1}^{N(h)} [Z_j(s_\ell + h) - Z_{j'}(s_\ell)]^2 - (\hat{\mu}_j - \hat{\mu}_{j'})^2, \tag{3.1}$$

where $N(h)$ is the number of lag-h differences and $\hat{\mu}_j$ is an estimated mean of the process Z_j, $j = 1, \ldots, k$. (The variables j and j' have to be in the same units for (3.1) to give meaningful results.) For a discussion of other, more robust, variogram estimators see Cressie and Hawkins (1980) and Cressie (1991).

We assume that the integer number n is even and that

$$\hat{\gamma}_{jj'}(h_i) = \hat{\gamma}_{j'j}(-h_i), \quad j,j' = 1,...,k, \quad i = 1,...,n. \tag{3.2}$$

We then fit permissible cross-variograms to the estimated values by, say, the weighted least squares method. That is, for a chosen set of positive weights $w_{ijj'}$, $i = 1,\dots,n$; $j,j' = 1,\dots,k$, we minimize the weighted least squares criterion

$$\min_{\boldsymbol{c},\boldsymbol{u},\boldsymbol{v}} \left\{ q(\boldsymbol{c},\boldsymbol{u},\boldsymbol{v}) = \sum_{j=1}^{k}\sum_{j'=1}^{k}\sum_{i=1}^{n} w_{ijj'} \left[\hat{\gamma}_{jj'}(h_i) - g_{jj'}(h_i)\right]^2 \right\}. \tag{3.3}$$

Here $g_{jj'}(\cdot) = c_{jj'} - f_{jj'}(\cdot)$, the functions $f_{jj'}$ are generated according to the formulas (2.16) and (2.17), subject to the non-negative definiteness condition and the condition that $g_{jj'}(\cdot)$ should be non-negative valued. (For $k = 2$, the functions $g_{jj'}(\cdot)$ and the non-negativity constraints are given by (2.24) and (2.25) respectively.) The optimization problem (3.3) is solved with respect to the variables $\boldsymbol{c} = [c_{jj'}]$ and vectors $\boldsymbol{u}, \boldsymbol{v}$ representing the corresponding elements of the matrices U^ℓ of (2.22). After an optimal solution $\tilde{\boldsymbol{c}}, \tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}$ of (3.3) is found, $\tilde{\boldsymbol{a}}$ and $\tilde{\boldsymbol{b}}$ are calculated using (2.23). The fitted cross-variograms are then generated according to the formulas

$$\tilde{g}_{jj'}(h) = \tilde{c}_{jj'} - \left[\sum_{\ell=1}^{m} \tilde{a}^{\ell}_{jj'} \cos(ht_\ell) - \tilde{b}^{\ell}_{jj'} \sin(ht_\ell)\right], \quad j,j' = 1,...,k. \tag{3.4}$$

A numerical solution of the optimization problem (3.3) requires application of nonlinear programming techniques. We used a method of iterative quadratic programming approximations (see Mayne and Polak (1982) for details). A FORTRAN code was developed that uses the subroutine QPROG from the IMSL library to solve the required quadratic programming problems. Since the objective function (3.3) involves fourth-order terms of the unknowns u^ℓ_ξ and v^ℓ_ξ, the Hessian matrix and gradient of the objective function are also given in terms of u^ℓ_ξ and v^ℓ_ξ. This entails provisioning of a non-zero vector of initial guess for solution of the problem. We tried random numbers $U \sim (0,1)$ as initial guess for various problems and found that the solution as well as the total number of iterations are hardly affected by the choice of the initial guess vector. Subsequently we used $1/(10\, m\, k)$ as the initial value for all u^ℓ_ξ and $v^\ell_\xi, \xi = 1,\dots,(k^2+k)/2$.

3.1. Examples

We demonstrate modeling of the cross-variograms with the help of two examples. The first one, involving two variables, is for a one-dimensional space while the second one is for two variables over a two- dimensional space. Variograms and cross-variograms for both examples were found using the same data set which comprises observations on moisture and temperature at 120 locations over a two- dimensional space. The observed values of the two variables were standardized using the sample means and the standard deviations of the respective variables. For the first example, the distances along the x-axis alone were used as the lags for calculating the experimental values of the cross-variograms.

3.1.1. Modeling over a one-dimensional space

The experimental cross-variograms were calculated using (3.1). The number of experimental variograms was 21 for moisture, 22 for temperature and 48 for their cross-variogram. All the weights, $w_{ijj'}$, $i = 1,\ldots,n$, $j,j' = 1, 2$, were selected as 1.0. The value of m was chosen to be 10 with $t_\ell = 0.0058\ell$, $\ell = 1,\ldots,10$. The objective function was set up as per (3.3) with the models $g_{jj'}(\cdot)$ given by (2.24). The objective function was minimized subject to the constraints (2.25). This problem involving 63 unknowns took 37 s on a Sun Sparc Center 2K. The vectors $\tilde{\boldsymbol{a}}$ and $\tilde{\boldsymbol{b}}$ were subsequently found using (2.23). The vectors $\tilde{\boldsymbol{a}}$, $\tilde{\boldsymbol{b}}$ and $\tilde{\boldsymbol{c}}$ are

$$\begin{aligned}
\tilde{\boldsymbol{a}}_{11} &= (0.019, 0.131, 0.367, 0.378, 0.167, 0.052, 0.027, 0.039, 0.066, 0.0517)',\\
\tilde{\boldsymbol{a}}_{22} &= (0.026, 0.117, 0.194, 0.096, 0.009, 0.00097, 0.005, 0.017, 0.0495, 0.0667)',\\
\tilde{\boldsymbol{a}}_{12} &= -(0.0014, 0.004, 0.008, 0.012, 0.01, 0.005, 0.003, 0.007, 0.02, 0.026)',\\
\tilde{\boldsymbol{b}}_{12} &= (0.022, 0.123, 0.266, 0.189, 0.038, 0, -0.011, -0.025, -0.054, -0.0526)'\\
\tilde{\boldsymbol{c}} &= (c_{11}, c_{22}, c_{12})' = (2.814, 2.346, 1.965)'.
\end{aligned}$$

Plots of the fitted models are placed as Figs. 1, 2 and 3.

3.1.2. Modeling over a two- dimensional space

The experimental variograms and cross-variograms were estimated in two directions (45 and 135°) with (3.1) modified to account for vector lags. For this problem, m was chosen as 25 and t_ℓ were found using $t_\ell = \ell(\Delta t), \ell = 1,\ldots,25$, with $\Delta t =$

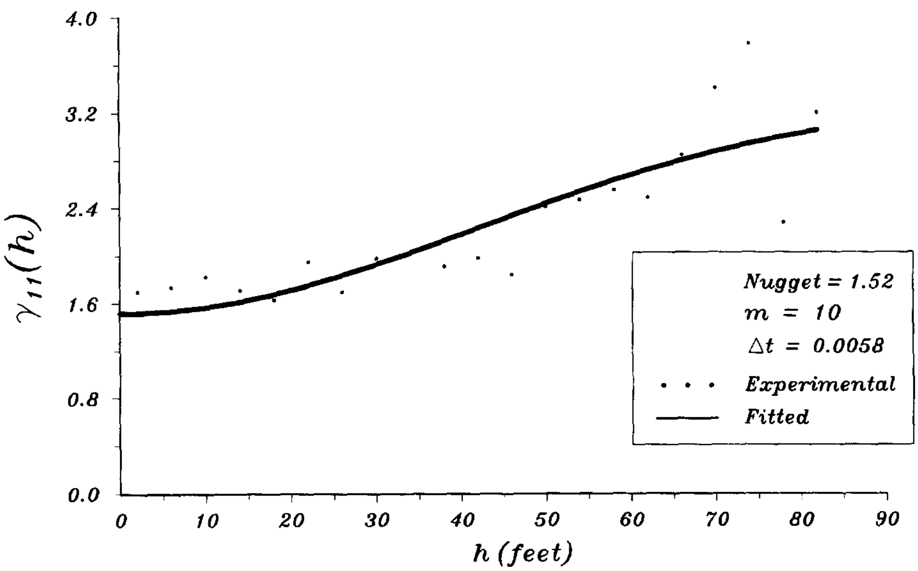

Fig. 1. Model for the moisture data over a one-dimensional space. For moisture, mean = 10.75, var = 37.05, skewness = 0.64, kurtosis = 2.212.

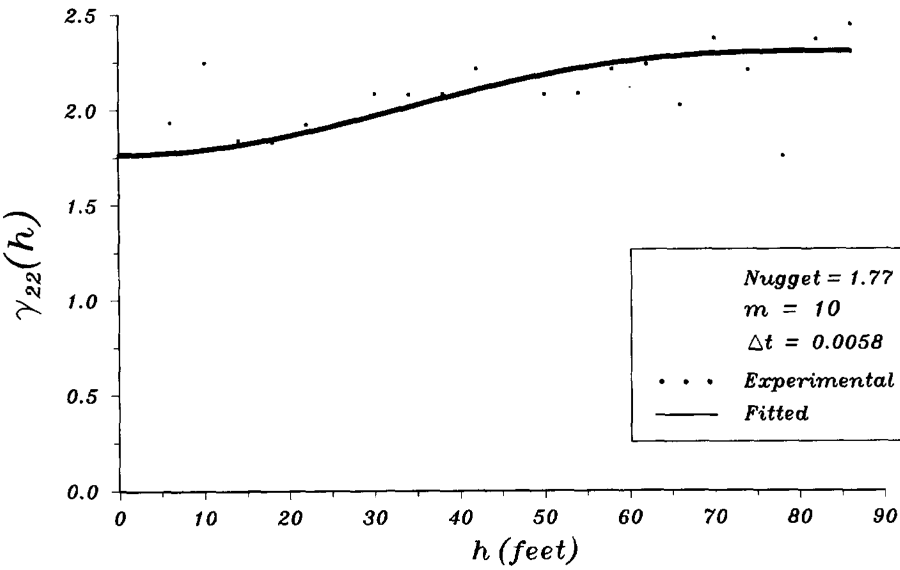

Fig. 2. Model for the temp. data over a one-dimensional space. For temp., sample mean = 37.95, var = 17.98, skewmess = 0.36, kurtosis = 1.72.

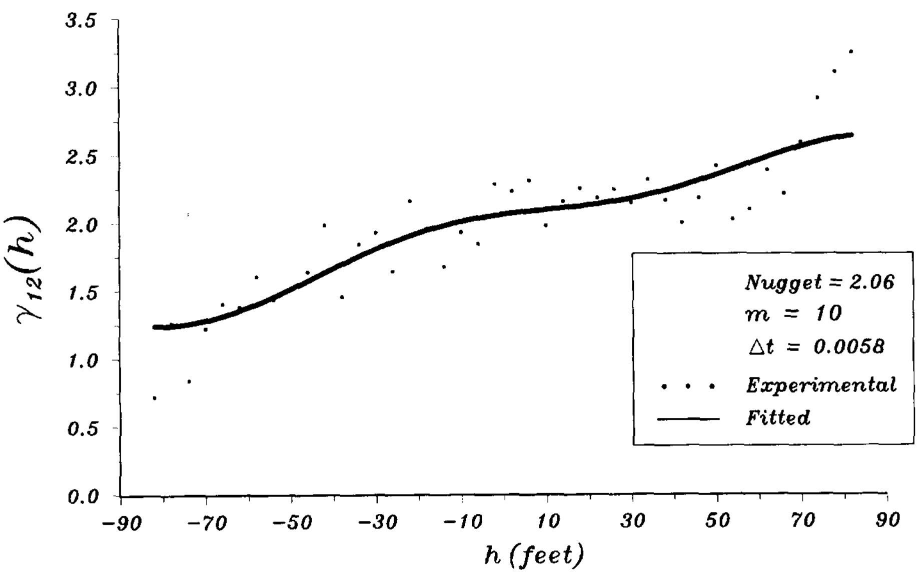

Fig. 3. Cross-Variogram model for moisture & temperature over a one-dimensional space.

0.01. The objective function was set up according to (3.3) with the models $g_{jj'}(\cdot)$ given by (2.33a). The lower triangular matrix $\boldsymbol{L}$ was initialized by using a 2×2 identity matrix. The objective function was then minimized subject to the non-negativity constraints (2.30). This problem with 81 unknowns took 32 s on a Sun Sparc Center 2K. The vector $\tilde{\boldsymbol{a}}$ was then found using (2.32) and is placed in Table 1. The vector

Table 1
Coefficients of the models fitted to the empirical cross-variograms of moisture and temperature over a two- dimensional space

ℓ	$\tilde{a}_{11}^{\ell}$	$\tilde{a}_{22}^{\ell}$	$\tilde{a}_{12}^{\ell}$
1	0.00000	0.00000	0.00000
2	0.00389	0.00025	0.00076
3	1.05423	0.02945	0.13985
4	0.11790	0.17190	−0.12689
5	0.00487	0.01828	−0.00935
6	0.00039	0.00103	−0.00062
7	0.00066	0.00124	−0.00086
8	0.00597	0.01061	−0.00762
9	0.02863	0.03831	−0.03252
10	0.07194	0.05187	−0.06060
11	0.09005	0.04561	−0.06356
12	0.03923	0.03075	−0.03424
13	0.01223	0.02235	−0.01624
14	0.00785	0.01215	−0.00955
15	0.02009	0.01324	−0.01585
16	0.08038	0.03069	−0.04808
17	0.09144	0.04681	−0.06271
18	0.04984	0.05224	−0.04877
19	0.04957	0.05263	−0.04951
20	0.05493	0.04806	−0.05032
21	0.02677	0.03031	−0.02803
22	0.01487	0.02341	−0.01841
23	0.01389	0.01143	−0.01222
24	0.01786	0.00442	−0.00812
25	0.00871	0.00258	−0.00411

$\tilde{c}$ and the matrix $\tilde{\boldsymbol{L}}$ are given by

$$\tilde{c} = (c_{11}, c_{22}, c_{12})' = (2.5197,\ 2.0411,\ 2.0692)',$$

$$\tilde{\boldsymbol{L}} = \begin{bmatrix} -1.280 & 0 \\ 0.571 & 0.610 \end{bmatrix}.$$

The models fitted to the two variograms are placed as Figs. 4 and 5, while the cross-variogram model is placed as Fig. 6. The model in Fig. 4 shows an obvious anisotropy. Tables 2 and 3 provide the values of the experimental and fitted variograms and cross-variogram respectively.

4. Parameters selection

The suggested approach of cross-variograms modeling involves assignment of numerical values to a number of parameters. Here we give rough guidelines for their selection.

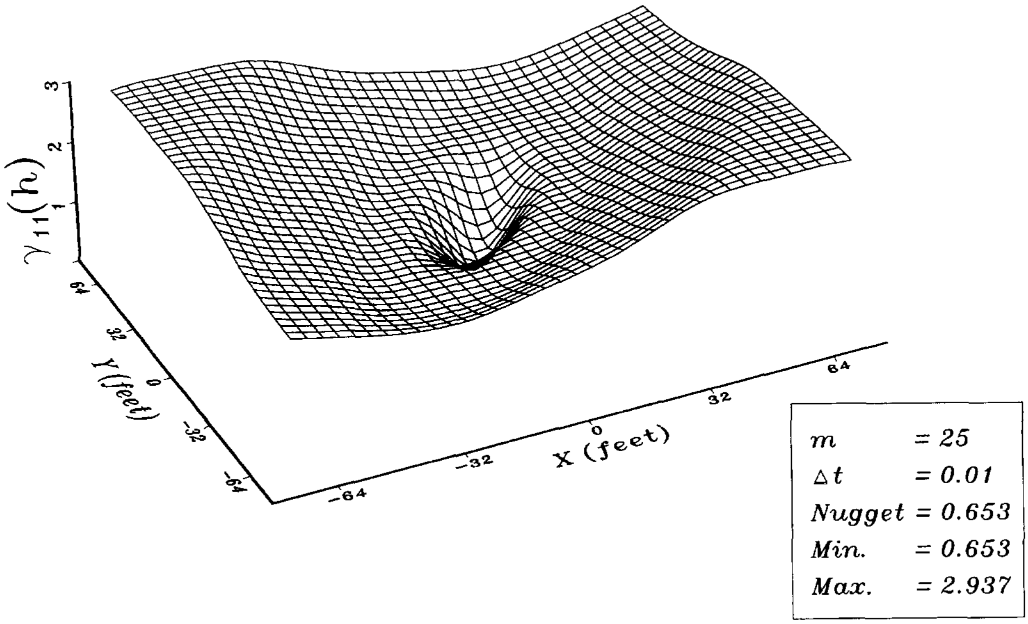

Fig. 4. Variogram surface for the moisture data. The sample satistics for the moisture data are mean = 10.75, variance = 37.05, skewness = 0.64, kurtosis = 2.212.

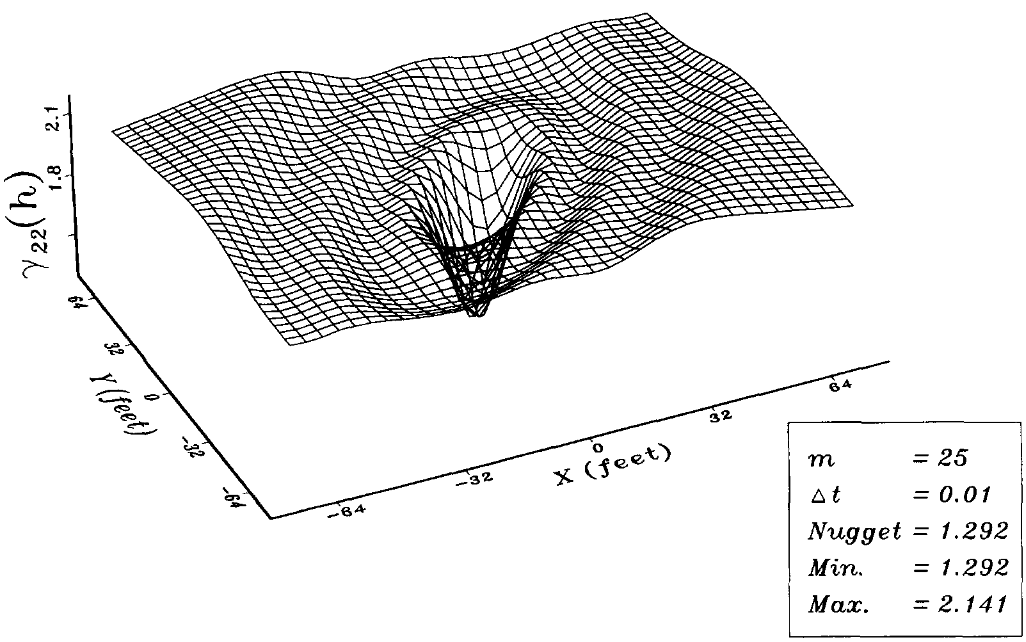

Fig. 5. Variogram surface for the temperature data. The sample statistics for the temperature data are mean = 37.95, variance = 17.98, skewness = 0.36, kurtosis= 1.718.

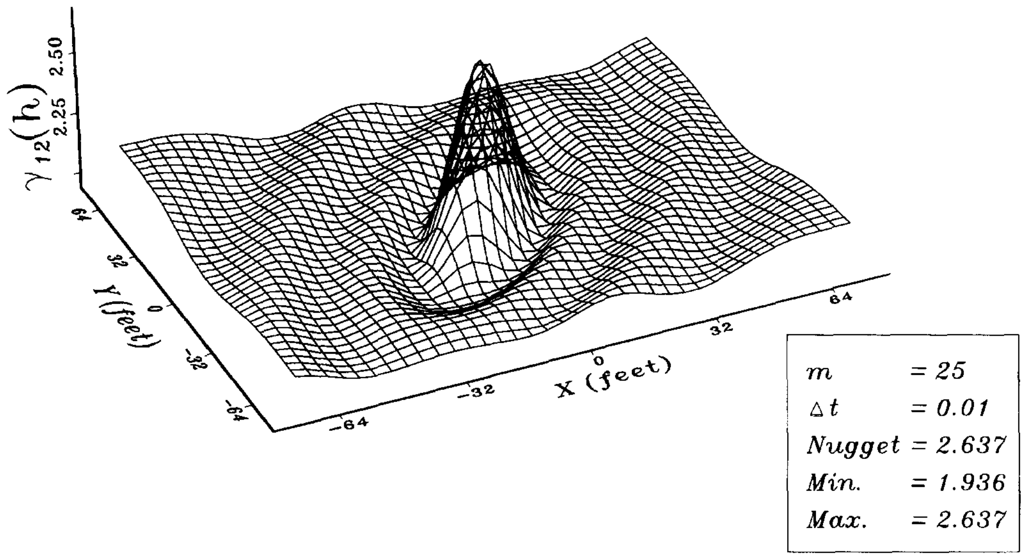

Fig. 6. Cross–Variogram surface for the moisture & temperature data over a two–dimensional space.

4.1. *Weights*

While fitting models to the empirical values, some sort of criterion for goodness of fit is needed. The criterion of weighted least squares (WLS), with weights chosen proportional to the error variance, is a common choice due to the ease of handling and the ability of this criterion to yield some desired properties of the estimators. Cressie (1985) has shown that variance of the variogram is a function of the number of pairs used in estimation of the empirical variogram as well as the variogram value itself. Because of the reliance of variances on the variograms, exact weights cannot be assigned a priori. One way of tackling this problem is to use an iterative scheme by starting with ordinary least squares. Shapiro and Botha (1991) have reported that the fit is hardly affected by the choice of these weights so ordinary least squares can be used by selecting all the weights to be 1.0.

4.2. *Effect of lags*

Since different data sets can have lags, $\boldsymbol{h}$, of different magnitudes, the choice of the frequencies, $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_m$, can become difficult. In order to overcome this problem, all the lags can be divided by the magnitude of the maximum lag in the data set. The resulting normalized lags would then range between zero and one, making the selection of $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_m$ comparatively easy.

4.3. *Discretizing intervals*

Selection of appropriate numbers m and $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_m$ is important since the objective function and the fitted models are quite sensitive to the choice of these numbers.

Table 2
Variograms of the moisture and temperature data

Lag	Moisture				Temperature			
	45° direction		135° direction		45° direction		135° direction	
	Exp.	Fit.	Exp.	Fit.	Exp.	Fit.	Exp.	Fit.
3.	0.525	0.672	0.709	0.732	1.112	1.305	0.932	1.350
6.	0.747	0.726	1.067	0.939	1.517	1.346	1.616	1.504
10.	1.237	0.845	1.011	1.284	1.889	1.434	2.127	1.753
14.	1.479	0.999	1.874	1.543	1.722	1.548	2.155	1.926
18.	1.245	1.168	1.761	1.650	2.033	1.671	2.096	1.970
22.	1.403	1.327	1.997	1.668	2.004	1.784	2.031	1.941
26.	1.717	1.461	2.141	1.697	2.075	1.875	1.778	1.925
30.	2.453	1.560	1.909	1.784	2.003	1.935	2.206	1.956
34.	1.685	1.622	2.164	1.907	1.672	1.965	1.947	2.007
38.	1.487	1.653	1.769	2.025	1.763	1.969	2.078	2.036
42.	1.736	1.664	1.547	2.121	1.778	1.958	2.437	2.031
46.	1.182	1.669	1.976	2.203	2.052	1.941	2.344	2.017
50.	1.152	1.677	2.283	2.289	2.151	1.928	2.277	2.021
54.	1.699	1.696	2.379	2.394	1.824	1.925	2.268	2.051
58.	1.497	1.730	2.277	2.519	1.698	1.934	2.543	2.091
62.	1.480	1.776	2.609	2.652	1.859	1.953	2.323	2.123
66.	1.764	1.832	2.690	2.770	2.063	1.978	2.339	2.139
70.	2.461	1.893	3.010	2.854	1.620	2.002	2.241	2.140
74.	1.749	1.953	3.934	2.899	2.224	2.022	1.968	2.132
78.	1.339	2.009	2.550	2.918	1.577	2.034	2.129	2.120
82.	1.612	2.060	2.849	2.926	2.080	2.037	2.114	2.106
86.	2.470	2.105	3.536	2.930	1.716	2.034	1.913	2.092
90.	1.876	2.146	3.020	2.934	1.972	2.027	2.018	2.078
94.	1.871	2.185	2.481	2.936	1.224	2.019	1.647	2.064
98.	1.198	2.224	2.712	2.936			1.372	2.049
102.			4.035	2.922				

We fitted models to the same data sets using different values of m and $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_m$ to observe the effect of their choice. It was observed that smoothness and the ability of the fitted models to chase the experimental values depend heavily on the choice of $\boldsymbol{t}_m$. For a given value of $\boldsymbol{t}_m$, the value of m was observed to have little effect on the fitted models. Since choice of the frequencies, $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_m$, is crucial, their selection can be made data dependent by including one additional unknown in the optimization problem. For the case of $d = 1$, consider using $t_\ell = \ell\alpha$, where α can be treated as an unknown interval in the frequency domain and its value can be found along with the vectors $\boldsymbol{c}$, $\boldsymbol{u}$ and $\boldsymbol{v}$ while optimizing (3.3). This procedure can also be used with the isotropic models (2.28) and (2.29) for $d = 2$ and $d = 3$ respectively. A similar methodology can be adopted while using the anisotropic models (2.26) and (2.27) with additional unknowns $\alpha_1, \ldots, \alpha_d$. The models (2.33a) and (2.33b) do not require additional unknowns since the requirement of varying the interval size is automatically fulfilled by the elements of the matrix $\boldsymbol{L}$. The suggested approach of

Table 3
Cross-variograms of the moisture and temperature data

	45° direction		135° direction		225° direction		315° direction	
Lag	Exp.	Fit.	Exp.	Fit.	Exp.	Fit.	Exp.	Fit.
3.	3.320	2.622	4.008	2.575	3.195	2.622	2.848	2.575
6.	2.991	2.579	2.837	2.414	3.081	2.579	2.535	2.414
10.	2.646	2.487	2.182	2.153	2.108	2.487	1.722	2.153
14.	2.036	2.367	1.384	1.976	2.718	2.367	1.865	1.976
18.	2.332	2.239	1.719	1.938	2.120	2.239	2.110	1.938
22.	1.677	2.121	2.145	1.985	1.962	2.121	1.873	1.985
26.	1.503	2.028	1.745	2.027	2.521	2.028	2.381	2.027
30.	1.751	1.967	2.094	2.024	2.214	1.967	1.819	2.024
34.	2.008	1.939	2.068	1.999	2.273	1.939	2.595	1.999
38.	1.427	1.939	1.592	1.992	2.373	1.939	2.339	1.992
42.	1.674	1.959	1.835	2.015	1.935	1.959	2.092	2.015
46.	2.307	1.985	1.932	2.050	2.050	1.985	2.126	2.050
50.	1.780	2.010	1.842	2.070	1.720	2.010	1.926	2.070
54.	1.523	2.026	1.396	2.066	1.975	2.026	1.823	2.066
58.	1.671	2.031	1.481	2.044	2.034	2.031	1.912	2.044
62.	1.980	2.026	1.575	2.020	1.935	2.026	2.407	2.020
66.	1.233	2.014	1.510	2.009	1.707	2.014	1.760	2.009
70.	0.923	2.002	1.286	2.014	2.107	2.002	2.227	2.014
74.	1.356	1.993	1.013	2.033	1.731	1.993	2.847	2.033
78.	2.202	1.991	1.107	2.059	2.761	1.991	2.598	2.059
82.	1.119	1.997	1.463	2.084	1.984	1.997	2.215	2.084
86.	1.781	2.009	2.049	2.105	2.120	2.009	3.051	2.105
90.			2.406	2.118			2.896	2.118
94.			3.099	2.125			3.965	2.125
98.			2.968	2.126				

estimating the value of α during the model fitting stage was tried on several data sets with different initial values of α. A unique value of the interval α could not be found with different choices of initial guess for a given data set, but the values of the objective function were found to be quite close. Subsequently, we tried initializing α by $5.0/(m \times h_{\max})$ with $h_{\max}$ being the magnitude of the maximum lag in the data set. (In case the lags are normalized as suggested in Section 4.2, $h_{\max}$ will be 1.0.) This method was found to result in good fits for values of m ranging between 5 and 50. Table 4 provides values of the objective function $q(\cdot)$ for various combinations of m and α for the data of example 1. Column 2 of this table contains the initial values of α used to start the optimization while column 3 has the corresponding optimal values of α. Note that each optimal value of α corresponds to a different set of the vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$.

The number of variables, k, and the number m determine the number of unknowns in the optimization problem. It may be desirable to keep the number of unknowns less than the total number of experimental values. This gives us a clue as to how the number m can be selected.

Table 4
Objective function of example 1 for different values of m and α

M	α initial	α final	Objective function	M	α initial	α final	Objective function
5	0.0010	0.0504	14.39	5	0.0100	0.0423	12.54
5	0.1000	0.1400	17.42	5	0.5000	0.3340	16.73
10	0.0010	0.1480	10.12	10	0.0100	0.0410	11.48
10	0.1000	0.1100	18.25	10	0.5000	0.4910	16.02
15	0.0010	0.0256	08.94	15	0.0100	0.0259	08.09
15	0.1000	0.0986	16.08	15	0.5000	0.4870	11.80
20	0.0010	0.1206	13.71	20	0.0100	0.0400	11.09
20	0.1000	0.0641	12.55	20	0.5000	0.4980	11.78
5	0.0116*	0.0325	09.77	10	0.0058*	0.0291	07.59
15	0.0039*	0.0320	07.94	20	0.0029*	0.0030	06.74
25	0.0023*	0.0029	05.96	30	0.0019*	0.0006	05.45
35	0.0017*	0.0024	05.50	40	0.0015*	0.0019	05.02
45	0.0013*	0.0032	04.93	50	0.0012*	0.0014	05.05

* denotes the initial values found by using $\alpha = 5/(m \times h_{\max})$.

5. Conclusions

In this article, we have suggested the use of integral transforms for cross-variograms modeling. Various forms of these transforms are then shown to meet the requirements like asymmetry and anisotropy of the fitted models. A parameterization of the unknowns based on Cholesky decomposition of the coefficient matrices is also introduced. This method ensures joint conditional negative definiteness of the fitted models for any number of variables without any need for additional constraints. Applicability of the suggested models along with the parameterization approach is demonstrated with examples for two variables over one- and two- dimensional spaces. The first example highlights the ability of the suggested functions to model asymmetry of the cross-variograms. The second example focuses on the ability of the suggested functions to model anisotropies of the variograms/cross-variograms. Effects of various modeling parameters on the fitted models are finally discussed and a procedure for the selection of those parameters is outlined.

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