Cross-covariance functions for multivariate random fields based on latent dimensions

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SUMMARY

The problem of constructing valid parametric cross-covariance functions is challenging. We propose a simple methodology, based on latent dimensions and existing covariance models for univariate random fields, to develop flexible, interpretable and computationally feasible classes of cross-covariance functions in closed form. We focus on spatio-temporal cross-covariance functions that can be nonseparable, asymmetric and can have different covariance structures, for instance different smoothness parameters, in each component. We discuss estimation of these models and perform a small simulation study to demonstrate our approach. We illustrate our methodology on a trivariate spatio-temporal pollution dataset from California and demonstrate that our cross-covariance performs better than other competing models.

Some key words: Asymmetry; Linear model of coregionalization; Nonseparability; Positive definiteness; Space and time; Stationarity.

1. INTRODUCTION

Consider a *p*-dimensional multivariate random field $Z(x) = \{Z_1(x), \ldots, Z_p(x)\}^T$ defined on a region $D \subset \mathbb{R}^q$. For example, $x = s \in \mathbb{R}^d$, $d \ge 1$, yields a multivariate spatial random field and $x = (s, t) \in \mathbb{R}^{d+1}$ a multivariate spatio-temporal random field, where *s* denotes a spatial location and *t* denotes time. If we assume that *Z* is Gaussian, we only need to describe its mean and cross-covariance functions. We focus on the characterization of the latter, that is,

$$\operatorname{cov}\{Z_i(x_1), Z_i(x_2)\} = C_{ii}(x_1, x_2), \tag{1}$$

for i, j = 1, ..., p and for all x_1 and x_2 in D. In order for (1) to be a valid cross-covariance function, the covariance matrix Σ of the random vector $\{Z(x_1)^T, ..., Z(x_n)^T\}^T \in \mathbb{R}^{np}$ must be positive definite for any positive integer n and any points $x_1, ..., x_n$ in \mathbb{R}^q . To ensure positive definiteness, one often specifies the covariance function to belong to a parametric family whose members are known to be positive definite. In recent years, there has been a growing interest in the construction of valid cross-covariance functions.

Separable cross-covariance functions (Mardia & Goodall, 1993) are defined by $C_{ij}(x_1, x_2) = \rho(x_1, x_2)a_{ij}$, where $A = \{a_{ij}\}$ is a $p \times p$ positive definite matrix and $\rho(\cdot, \cdot)$ is a valid correlation

function. This model is not flexible enough to handle complex relationships between processes. For example, for two locations x_1 and x_2 , the cross-covariance function between components measured at each location always has the same shape regardless of the relative displacement of the locations.

The linear model of coregionalization for stationary processes (Goulard & Voltz, 1992; Wackernagel, 2003; Gelfand et al., 2004) implies that the cross-covariance function is

$$C_{ij}(x_1 - x_2) = \sum_{k=1}^{r} \rho_k(x_1 - x_2) a_{ik} a_{jk},$$

for an integer $1 \le r \le p$, where $A = \{a_{ij}\}$ is a $p \times r$ full rank matrix and $\rho_k(\cdot)$ are valid stationary correlation functions. One can view the matrix A as a principal component transformation, although it is too restrictive to assume that A does not change with $x_1 - x_2$. A spatially varying linear model of coregionalization, however, has too many parameters. When r = 1, the separable model is obtained.

The kernel convolution method (Ver Hoef & Barry, 1998) defines

$$C_{ij}(x_1, x_2) = \int_{\mathbb{R}^q} \int_{\mathbb{R}^q} k_i(x_1 - \tau_1) k_j(x_2 - \tau_2) \rho(\tau_1 - \tau_2) d\tau_1 d\tau_2,$$

where the k_i are square integrable kernel functions and $\rho(\cdot)$ is a valid stationary correlation function. This approach assumes that all the spatial processes $Z_i(x)$, for i = 1, ..., p, are generated by the same underlying process, which is very restrictive because it imposes strong dependence between all the processes $Z_i(x)$. Overall, this model and its parameters lack interpretability and, except for some special cases, it requires Monte Carlo integration.

The covariance convolution for stationary spatial processes (Gaspari & Cohn, 1999; Majumdar & Gelfand, 2007) yields

$$C_{ij}(s) = \int_{\mathbb{R}^d} C_i(s-\tilde{s})C_j(\tilde{s})d\tilde{s},$$

where C_i are valid stationary covariance functions. The motivation and interpretation of the resulting cross-dependency structure is rather unclear. Although some closed-form expressions exist, this method usually requires Monte Carlo integration.

The problem of constructing valid parametric cross-covariance functions is challenging, as mentioned recently by Zhang (2007, p. 127). Our goal in this article is to introduce a general class of models that is interpretable, flexible and computationally feasible.

We propose an approach based on existing covariance models for univariate (p = 1) random fields; see, for instance, Cressie & Huang (1999), Gneiting (2002) and Gneiting et al. (2007). The key idea is to represent a vector's components as points in a k-dimensional space, for an integer $1 \le k \le p$, say, the *i*th component can be represented as $\xi_i = (\xi_{i1}, \ldots, \xi_{ik})^T$. Then, based on these latent dimensions, (1) becomes a covariance with arguments from \mathbb{R}^{q+k} , $C\{(x_1, \xi_i), (x_2, \xi_j)\}$. Consequently, the matrix Σ above is guaranteed to be positive definite because its entries are defined through a valid covariance. In fact for any x_1, x_2 there exists $C_{x_1,x_2}(\cdot)$ such that $C_{ij}(x_1, x_2) = C_{x_1,x_2}(\xi_i - \xi_j)$, for some $\xi_i, \xi_j \in \mathbb{R}^k$ (Perrin & Schlather, 2007). Generally, instead of specifying the ξ_i s, we can treat them as parameters. Alternatively, one can use only distances between a vector's components, $\delta_{ij} = ||\xi_i - \xi_j||$, the so-called component isotropic models. Overall, the modelling idea is similar to multi-dimensional scaling (Cox & Cox, 2000) with latent distances δ_{ij} s, where for fixed locations x_1 and x_2 , larger δ_{ij} s are translated to smaller crosscorrelations between the *i*th and *j*th components of a vector. In the rest of this article, we assume that the covariance function is stationary in space and time, namely, $C_{ij}(x_1, x_2) = C_{ij}(x_1 - x_2)$. We develop flexible cross-covariance functions capable of modelling complex nonseparable and asymmetric structures for multivariate random fields.

2. Cross-covariance functions

2.1. Background and main results

Separability means that the cross-covariance structure factors into purely space-time and purely vector component terms, and so allows computationally efficient estimation. Consequently, separable covariance models have been popular even in situations in which they are not physically justifiable. Families of nonseparable space-time covariance functions, that is, when the covariance function is not a product of a purely temporal function and a purely spatial function, were studied by several authors; for instance, Cressie & Huang (1999), Gneiting (2002) and Gneiting et al. (2007). Here we propose an explicit expression for the variable and space-time nonseparable cross-covariance function; see Proposition 1 below. More complex cross-covariance functions can be built by using results of Proposition 2.

Recall that a real and positive function φ is completely monotone if and only if its *n*th derivative $\varphi^{(n)}$ satisfies $(-1)^n \varphi^{(n)}(t) \ge 0$, for all $n \in \mathbb{N}$. Based on Gneiting (2002), the following covariance function is positive definite in space-time lags $(h, u) \in \mathbb{R}^{d+1}$:

$$C(h, u) = \frac{\sigma^2}{\{\psi_1(|u|^2)\}^{d/2}} \varphi_1\left\{\frac{\|h\|^2}{\psi_1(|u|^2)}\right\}$$

where $\varphi_1(t)$, $t \ge 0$, is a completely monotone function, $\psi_1(t)$, $t \ge 0$, is a positive function with completely monotone derivative and σ^2 is a variance parameter. We extend the results of Gneiting (2002) to include a third argument reserved for the representation of the vector's components with the following family of cross-covariance functions.

PROPOSITION 1. Suppose that $\varphi_1(t)$, $t \ge 0$, is a completely monotone function, and let $\psi_i(t)$, $i = 1, 2, t \ge 0$, be positive functions with a completely monotone derivative. Then

$$C(h, u, v) = \frac{\sigma^2}{\left[\psi_1\left\{\frac{|u|^2}{\psi_2(||v||^2)}\right\}\right]^{d/2} \{\psi_2(||v||^2)\}^{1/2}} \varphi_1\left[\frac{\|h\|^2}{\psi_1\left\{\frac{|u|^2}{\psi_2(||v||^2)}\right\}}\right], \quad (h, u, v) \in \mathbb{R}^{d+1+k},$$
(2)

is a stationary covariance function.

The proof is in the Appendix. It is known that for positive definite functions, the following properties are true. Any finite linear combination of positive definite functions with nonnegative coefficients is positive definite. The finite product of positive definite functions is also positive definite. A continuous function that is the limit of a sequence of positive definite functions is itself positive definite; for example, $\exp{\{\psi(x)\}}$ is positive definite if $\psi(x)$ is positive definite. In addition, we have the following result, the proof of which is in the Appendix.

PROPOSITION 2. Let $C_i(h, u, v)$ (i = 1, ..., L) be valid stationary covariance functions on \mathbb{R}^{d+1+k} . Then

$$C(h, u, v) = \prod_{i=1}^{L} C_i(h \lor 0, u \lor 0, v \lor 0), \quad (h, u, v) \in \mathbb{R}^{d+1+k},$$
(3)

where $a \lor 0$ means that the argument can be replaced by 0, is a stationary covariance function.

Type of separability	Form	Functions to be equal to a constant
Full	$C_1(h)C_2(u)C_3(v)$	ψ_1, ψ_2, ψ_3
Space-time partial	$C_1(h, v)C_2(u, v)$	ψ_1
Space-variable partial	$C_1(h, u)C_2(u, v)$	ψ_3,ψ_4
Time-variable partial	$C_1(h, u)C_2(h, v)$	ψ_2,ψ_4
Space	$C_1(h)C_2(u, v)$	ψ_1,ψ_3
Time	$C_1(u)C_2(h, v)$	ψ_1,ψ_2
Variable	$C_1(v)C_2(h, u)$	ψ_2, ψ_3, ψ_4

 Table 1. Special cases of the cross-covariance model (4)

There are alternative ways to define a model for the covariance function of a random field. Under certain conditions, there exists a spectral density function associated with the spectral distribution function. By definition, the spectral density for the *i*th and *j*th components is

$$f_{ij}(\omega_1,\omega_2) = \frac{1}{(2\pi)^{d+1}} \int_{\mathbb{R}^1} \int_{\mathbb{R}^d} \exp(-\iota h^{\mathsf{T}}\omega_1) \exp(-\iota u\omega_2) C_{ij}(h,u) dh du,$$

where $\iota = (-1)^{1/2}$. It is known (Yaglom, 1987) that cross-spectral densities $f_{ij}(\omega_1, \omega_2)$ have to form a Hermitian and positive definite matrix for almost all $(\omega_1, \omega_2) \in \mathbb{R}^{d+1}$. If $C_{ij}(h, u) =$ $C(h, u, v_{ij})$ as proposed, then $f_{ij}(\omega_1, \omega_2) = C_{\omega_1, \omega_2}(v_{ij})$, where $C_{\omega_1, \omega_2}(\cdot)$ is a valid covariance function for almost all $(\omega_1, \omega_2) \in \mathbb{R}^{d+1}$ by the Lemma A1 in the Appendix and Theorem 1 from Gneiting (2002). Since $C_{\omega_1,\omega_2}(v_{ij})$ (i, j = 1, ..., p) form a positive definite matrix, so do $f_{ii}(\omega_1, \omega_2)$ for almost all $(\omega_1, \omega_2) \in \mathbb{R}^{d+1}$.

2.2. Cross-covariances with identical autocovariances

A stationary covariance function is isotropic if it is rotation and translation invariant. A fully isotropic space-time multivariate random field, $Z_i(s, t)$, (i = 1, ..., p), $s \in \mathbb{R}^d$, $t \in \mathbb{R}^1$, is isotropic for every argument, that is, $cov\{Z_i(s_1, t_1), Z_j(s_2, t_2)\} = C_{ij}(||s_1 - s_2||, |t_1 - t_2|) =$ $C(||s_1 - s_2||, |t_1 - t_2|, ||\xi_i - \xi_i||)$. In other words, the processes for each component i have the same isotropic covariance function with respect to space and time, that is, they have identical autocovariances. We utilize a fully isotropic model as a building block for more complex structures; see below and $\S 2 \cdot 3$.

Combining the results in Propositions 1 and 2, we propose the following flexible model of stationary cross-covariance functions on \mathbb{R}^{d+1+k} :

$$C(h, u, v) = \frac{\sigma^2}{\left[\psi_1\left\{\frac{|u|^2}{\psi_4(||v||^2)}\right\}\right]^{d/2} \{\psi_2(||v||^2)\}^{1/2} \{\psi_3(||h||^2)\}^{k/2} \{\psi_4(||v||^2)\}^{1/2}} \times \varphi_1\left[\frac{||h||^2}{\psi_1\left\{\frac{|u|^2}{\psi_4(||v||^2)}\right\}}\right] \varphi_2\left\{\frac{|u|^2}{\psi_2(||v||^2)}\right\} \varphi_3\left\{\frac{||v||^2}{\psi_3(||h||^2)}\right\}.$$
(4)

The arguments in (4) can be interchanged while preserving the validity of the resulting covariance function. Many valid covariance models can be constructed based on (4) and the functions $\varphi(t)$ and $\psi(t)$ listed in tables 1 and 2 of Gneiting (2002, p. 591). The proposed model (4) is fully nonseparable and next we demonstrate how to make it flexible enough to handle all special cases of separability. We assume that each ψ_i has a tuning parameter that at some special value yields a constant function. Table 1 summarizes special cases of the cross-covariance model (4).

Marginally (v = 0), nonseparable space-time covariance models have been used extensively and the choice of particular functional forms of φ_i (i = 1, 2) and ψ_j (j = 1, 3) can be guided by

empirical variograms or covariograms, or by statistical tests (Li et al., 2007). The choice of other functions is more arbitrary mainly because of the nature of latent observations and the fact that the number of components is far less than the number of locations in most practical applications. Therefore, one should settle with the most computationally convenient functional forms. We advise trying several candidate functions to compare the fit when p is large. Knowledge about forms of separability can suggest simplifications of (4); see Table 1. More specifically, consider the functions $\varphi_i(t) = \exp(-c_i t^{\gamma_i})$ (i = 1, ..., 3) and $\psi_j(t) = (a_j t^{\alpha_j} + 1)^{\beta_j}$ (j = 1, ..., 4) proposed by Gneiting (2002, p. 593). For a multivariate spatio-temporal random field, we obtain the following cross-covariance model:

$$C(h, u, v) = \sigma^{2} \left(\left[a_{1} \left\{ |u|^{2} / (a_{4} ||v||^{2\alpha_{4}} + 1)^{\beta_{4}} \right\}^{\alpha_{1}} + 1 \right]^{\beta_{1} d/2} \right)^{-1} \\ \times \left\{ (a_{2} ||v||^{2\alpha_{2}} + 1)^{\beta_{2}/2} (a_{3} ||h||^{2\alpha_{3}} + 1)^{\beta_{3} k/2} (a_{4} ||v||^{2\alpha_{4}} + 1)^{\beta_{4}/2} \right\}^{-1} \\ \times \exp \left(- \frac{c_{1} ||h||^{2\gamma_{1}}}{\left[a_{1} \left\{ |u|^{2} / (a_{4} ||v||^{2\alpha_{4}} + 1)^{\beta_{4}} \right\}^{\alpha_{1}} + 1 \right]^{\beta_{1}\gamma_{1}}} - \frac{c_{2} |u|^{2\gamma_{2}}}{(a_{2} ||v||^{2\alpha_{2}} + 1)^{\beta_{2}\gamma_{2}}} - \frac{c_{3} ||v||^{2\gamma_{3}}}{(a_{3} ||h||^{2\alpha_{3}} + 1)^{\beta_{3}\gamma_{3}}} \right),$$
(5)

where $c_i > 0, 0 < \gamma_i \le 1$ for i = 1, ..., 3, and $a_j > 0, 0 < \alpha_j, \beta_j \le 1$ for j = 1, ..., 4. We set $d=2, k=1, \sigma^2=1, c_i=0.01, \gamma_i=1, a_j=0.07, \alpha_j=1$, and vary β_j . Figure 1 depicts contours of C(h, u, v) as a function of ||h||, |u| and |v|, for ||h||, $|u| \in [0, 12]$ and |v| = 0, 3.02, 4.27. The contour lines are such that the next line is the current one times 1.2 starting from 0.1. The choices of $\beta_i \in \{0, 1\}$ correspond to four cases from Table 1: full separability, that is all $\beta_i = 0$; space separability, that is only $\beta_2 = 1$; space-time partial separability, that is β_2 and β_3 are 1; and nonseparability, that is all $\beta_i = 1$. The choice of v_i s is such that $C(0, 0, v_1)/C(0, 0, v_2) = C(0, 0, v_2)/C(0, 0, v_3) = \sqrt{12}$, which makes the contour lines in the case of full separability move in a proportional fashion. Therefore, visually, all the cases can be assessed as deviations from proportionality as in full separability. We shall now describe separability with respect to space. Separability with respect to time and to variable can be deduced similarly. Fix h_1 , h_2 . For space separability, C(h, u, 0) and C(h, 0, v) are each separable, hence $C(h_1, u, v)/C(h_2, u, v) = \Delta_{12}$ for any u, v. For space-time partial separability, C(h, u, 0)is separable but C(h, 0, v) is nonseparable, thus $C(h_1, u, v)/C(h_2, u, v) = \Delta_{12}(v)$ is a function of v but not u. For nonseparability, C(h, u, 0) and C(h, 0, v) are each nonseparable, hence $C(h_1, u, v)/C(h_2, u, v) = \Delta_{12}(u, v)$ is a function of v and u.

2.3. Cross-covariances with different autocovariances

For the case where for each component *i* the processes have different isotropic covariance functions with respect to space and time, we propose using the following cross-covariance functions. Consider independent univariate random fields $W_l(s, t, \xi)$ (l = 1, ..., L), with covariance function $\operatorname{cov}\{W_l(s_1, t_1, \xi_1), W_l(s_2, t_2, \xi_2)\} = C_l(||s_1 - s_2||, |t_1 - t_2|, ||\xi_1 - \xi_2||)$. We model the multivariate random field *Z* with a linear model of coregionalization based on latent dimensions, that is

$$Z_i(s,t) = \sum_{l=1}^{L} a_{il} W_l(s,t,\xi_i) \quad (i=1,\ldots,p),$$
(6)

with constant coefficients a_{il} . Thus, the cross-covariance function of (6) is

$$\operatorname{cov}\{Z_i(s_1, t_1), Z_j(s_2, t_2)\} = \sum_{l=1}^{L} a_{il} a_{jl} C_l(\|s_1 - s_2\|, |t_1 - t_2|, \|\xi_i - \xi_j\|) \quad (i, j = 1, \dots, p).$$



Fig. 1. Graphs showing the contour lines of the cross-covariance function (5) for the following special cases: full, space, space-time partial and nonseparability (columns) for $||h||, |u| \in [0, 12]$ and |v| = 0, 3.02, 4.27 (rows).

A special case of (6) is to model Z by

$$Z_i(s, t) = a_{i1}W(s, t, \xi_i) + a_{i2}W_i(s, t),$$

where $W_i(s, t)$ (i = 1, ..., p) are independent univariate random fields. Therefore

$$\operatorname{cov}\{Z_{i}(s_{1}, t_{1}), Z_{j}(s_{2}, t_{2})\} = \begin{cases} a_{i1}^{2}C(\|s_{1} - s_{2}\|, |t_{1} - t_{2}|, 0) + a_{i2}^{2}C_{i}(s_{1} - s_{2}, t_{1} - t_{2}) & (i = j), \\ a_{i1}a_{j1}C(\|s_{1} - s_{2}\|, |t_{1} - t_{2}|, \|\xi_{i} - \xi_{j}\|) & (i \neq j), \end{cases}$$

$$(7)$$

where the C_i s are covariance functions for the W_i s.

The covariance between Z_i and Z_j can be negative when the coefficients a_{i1} and a_{j1} have different signs. Furthermore, the space-time covariance structure of each component of the multivariate random field is allowed to be different. For instance, different smoothnesses can be obtained by using different Matérn covariances C_i (Matérn, 1986) as long as W is the smoothest random field.

2.4. Asymmetric cross-covariances

Full symmetry happens when $C_{ij}(h, u) = C_{ij}(-h, u) = C_{ij}(h, -u) = C_{ij}(-h, -u)$. However, environmental, atmospheric and geophysical processes are often influenced by prevailing winds or ocean currents, which are incompatible with the assumption of full symmetry. Asymmetric behaviour is observed when the response of one variable affects another variable delayed in time. Here we can distinguish between the following types of asymmetry:

Type 1. Occurs when there is a time lag in a correlation between variables, so that $C_{ij}(h, u) = \tilde{C}_{ij}(h, u - \Delta_{ij})$, where $\tilde{C}_{ij}(h, u)$ is fully symmetric. We propose the following model:

$$C_{ij}^{(1)}(h, u) = C(h, u - \lambda_{\xi}^{\mathrm{T}}(\xi_i - \xi_j), \xi_i - \xi_j),$$

where λ_{ξ} is a k-vector and the shift $\Delta_{ij} = \lambda_{\xi}^{T}(\xi_{i} - \xi_{j})$ is such that $\operatorname{argmax}_{u} C_{ij}^{(1)}(h, u) = -\operatorname{argmax}_{u} C_{ji}^{(1)}(h, u) = \Delta_{ij}$, where $\Delta_{ij} = 0$ if and only if $\lambda_{\xi} = 0$ or i = j.

Type 2. Multivariate version of the model considered by several authors (Stein, 2005; Cox & Isham, 1988). We propose the following model:

$$C_{ij}^{(2)}(h, u) = C(h - \gamma_h u, u, \xi_i - \xi_j - \gamma_{\xi} u),$$

where the *d*-vector γ_h and the *k*-vector γ_{ξ} are velocities responsible for the lack of symmetry. For each *i* and *j*, $\operatorname{argmax}_h C_{ij}^{(2)}(h, u)$ depends on *u* and is equal to 0 if and only if either u = 0 or $\gamma_h = 0$; similarly, for each *h*, $\operatorname{argmax}_{i,j} C_{ij}^{(2)}(h, u)$ depends on *u* and is achieved when i = j if and only if either u = 0 or $\gamma_{\xi} = 0$. This model is spatially anisotropic when $u \neq 0$.

The combination of Type 1 and Type 2 is possible. We illustrate Type 1 and Type 2 using (5). We fix $h_2 = 0$, such that h is univariate and $h = h_1$, and we let p = 2, k = 1, $\xi_1 = 0$ and $\xi_2 = 3$. For Type 1, $\lambda_{\xi} = -0.5$ and for Type 2, $\gamma_h = 0.3$ and $\gamma_{\xi} = -0.5$. We vary β s and let $u, h \in [-10, 10]$. Figure 2 depicts $C_{11}^{(k)}(h, u), C_{12}^{(k)}(h, u)$ and $C_{21}^{(k)}(h, u)$ (k = 1, 2) for various β s and vs. The lack of symmetry is apparent.

3. ESTIMATION

Our key idea for constructing valid parametric cross-covariance functions is to represent a vector's components as points in a k-dimensional space, for an integer $1 \le k \le p$, say the *i*th component is represented as $\xi_i = (\xi_{i1}, \ldots, \xi_{ik})^T$. Here we assume that the covariance functions depend only on the distances between a vector's components, $\delta_{ij} = ||\xi_i - \xi_j||$. There are two approaches to estimating parameters associated with the vector's components: the first is to treat the ξ_i s as parameters and the second is to treat the δ_{ij} s as parameters.

Euclidean distance is invariant under translation, rotation and reflection about the origin, therefore we can constrain the configuration built by the ξ_i s to be centered and to be in principal axis orientation, for an integer $1 \le k \le p$:

$$\xi_{1j} \ge 0, \quad \sum_{i=1}^{p} \xi_{ij} = 0, \quad \sum_{i=1}^{p} \xi_{ij} \xi_{il} = 0 \quad (j, l = 1, \dots, k; l \neq j).$$
 (8)

The number of free parameters is kp - k(k+1)/2 and for k it is less than the totalnumber of all pairwise differences, <math>p(p-1)/2. For example, if p = 3 and k = 2, then three free parameters can be chosen as $\xi_{11}, \xi_{12} > 0, \xi_{21}$ and the other parameters can be derived from $\xi_{31} = -(\xi_{11} + \xi_{21}), \xi_{22} = -(2\xi_{11}\xi_{12} + \xi_{12}\xi_{21})/(2\xi_{21} + \xi_{11}), \xi_{32} = (\xi_{11}\xi_{12} - \xi_{21}\xi_{12})/(2\xi_{21} + \xi_{11})$. The positivity constraints are easy to handle by the reparameterization $\xi_{1j} = \exp(\chi_{1j})$. Then an unconstrained optimization can be applied to a criterion function $\mathcal{L}(\xi_1, \ldots, \xi_p)$; for example, least squares, maximum likelihood or composite likelihood; see Apanasovich et al. (2008) and a technical report by Bevilacqua, Gaetan, Mateu and Porcu from the University of Jaume I and references therein. The solution may not be unique even up to the order of axes. The order of axes can be constrained by, say, $\xi_{1j} > \xi_{1j-1}$ ($j = 2, \ldots, k$). Constraints on the parameters can be



Fig. 2. Graphs showing contour lines of asymmetric cross-covariance functions of Type 1 (a) and Type 2 (b) for various values of β and v = 0, 3, -3.

defined by specifying a function of these parameters to be maximized. For example, in the event that these constraints are a set of functions set equal to zero, the negative of the sum of squares of these functions serves as the appropriate function. The constraint function in the context of (8) without the inequality constraint on the reflection about the origin is

$$\mathcal{C}(\xi_1,\ldots,\xi_p) = -\frac{1}{2}\sum_{j=1}^k \left(\sum_{i=1}^p \xi_{ij}\right)^2 - \frac{1}{2}\sum_{j=1}^{k-1}\sum_{l=j+1}^k \left(\sum_{i=1}^p \xi_{ij}\xi_{il}\right)^2.$$

The parameters are estimated by

$$\operatorname{argmax}_{\xi_1,\ldots,\xi_p} \{ \mathcal{L}(\xi_1,\ldots,\xi_p) + \mathcal{C}(\xi_1,\ldots,\xi_p) \}.$$

In addition, one can use any variable selection criterion to choose the best value of k.

Alternatively, one can treat the elements δ_{ij} of the distance matrix as parameters. In this case the estimators of δ_{ij} are obtained by a constrained optimization method, where constraints come from the fact that δ_{ij} must form a valid distance matrix. Another option is to introduce measures of dissimilarities d_{ij} , such that $d_{ij} \ge 0$ and $d_{ij} = d_{ji}$ (i = 1, ..., p; j = 1, ..., k). The criterion function is evaluated at δ_{ij} s, which form a valid distance matrix, closest to $D = \{d_{ij}\}$, obtained as a solution of a classical multi-dimensional scaling problem, that is, minimizing $\sum_{ij} (d_{ij} - \delta_{ij})^2$. Here as well, one can use any variable selection criterion to choose the best value of k. In practice one would rarely pick $k > k^*$, where k^* is the smallest integer such that the number of parameters reserved for ξ_i s is greater or equal to the number of parameters reserved for the pairwise distances, specifically, $k^* = p/2$ or (p - 1)/2 for p even or odd, respectively.

The choice of the parameterization scheme is driven by the computational convenience and the modelling framework. Parameterization with respect to the coordinates produces a simpler criterion function to be maximized due to the fact that constraints on the coordinates are better defined analytically than constraints on the distances for k > 2. Moreover, the reduction of the number of free parameters when lowering k corresponds to the actual reduction of the number of parameters to be estimated only when using coordinates as parameters. However, parameterization with respect to the distances is more attractive for a Bayesian framework, where dissimilarities d_{ij} are assumed to follow truncated normal distributions, $d_{ij} \sim N(\delta_{ij}, \sigma^2)I(d_{ij} > 0)$, for $i \neq j$, where " $I(\cdot)$ is an indicator function.

4. MONTE CARLO SIMULATIONS

In our numerical work, we use the following routine for the sake of computational stability. Let θ be the collection of unknown parameters other than ξ_i s or δ_{ij} s. Iterate two steps until convergence: first, maximize the likelihood function with respect to θ , given the values of ξ_i s or δ_{ij} s from the previous iteration; second, estimate ξ_i s or δ_{ij} s using any method described previously given the values of θ obtained at the first step. We use zeros as the initial guess for ξ_i s and δ_{ij} s.

In the first simulation study, we address the issue of computational feasibility of the proposed method. We generate samples from a zero-mean *p*-dimensional spatial Gaussian random field. We use the following cross-correlation function $corr{Z_i(s_1), Z_j(s_2)}$ based on (7):

$$C_{ij}(\|h\|) = C(\|h\|, \|\xi_i - \xi_j\|)$$

= $\frac{\sigma_i \sigma_j}{\|\xi_i - \xi_j\| + 1} \exp\left\{\frac{-\alpha \|h\|}{(\|\xi_i - \xi_j\| + 1)^{\beta/2}}\right\} + \tau^2 I(i = j)I(\|h\| = 0),$ (9)

for i = 1, ..., p, where $h = s_1 - s_2$ and τ is a nugget effect. The parameters to be estimated are μ_i , means of the process, $\alpha > 0$, $\beta \in [0, 1]$, $\sigma_i > 0$, $\tau \ge 0$, $\xi_i \in \mathbb{R}^k$ or $\delta_{ij} \in \mathbb{R}^+$, k < p, subject to the constraints discussed in § 3, for i = 1, ..., p. We set p = 3 and simulate ξ_i s from a $[0, 1] \times [0, 1]$ square. We choose $\mu_i = 0$, $\alpha = 1$, $\beta = 1$, $\sigma_i = 1$, $\tau = 0.3$. Define $\theta = (\{\mu_i\}_{i=1,...,p}, \{\sigma_i\}_{i=1,...,p}, \alpha, \beta, \tau)$. We generate n = 150 points whose spatial locations were selected at random from the $[0, 10] \times [0, 10]$ square.

First, we compare the different ways to estimate the parameters responsible for the crosscorrelation. We fix k = 2 and apply the three methods outlined in § 3: unconstrained optimization using free parameters, ξ_{11} , ξ_{12} and ξ_{21} ; constrained optimization where nonlinear constraints are introduced through the penalty term; and constrained optimization treating δ_{ij} s as parameters with multi-dimensional scaling as the intermediate step. In 98% of the simulated samples, the same estimates of θ and $\|\xi_i - \xi_j\|$ s from the three methods listed above were produced. The number of iterations in the two-step procedure was the same for all methods and the unconstrained

Parameter	Separable		k = 1		k = 2	
	AB	SD	AB	SD	AB	SD
τ	0.19	0.09	0.01	0.05	0.01	0.05
α	0.07	0.07	0.10	0.12	0.10	0.11
β	_	_	0.13	0.28	0.08	0.24
	Wave AB	Wave SD	Wave AB	Wave SD	Wave AB	Wave sD
μ_i	0.01	0.24	0.01	0.24	0.00	0.24
σ_i	0.28	0.13	0.04	0.09	0.03	0.09
$\ \xi_i - \xi_j\ $	_	_	0.10	0.32	0.06	0.31
Range for corr _i	0.18	0.27	0.19	0.29	0.16	0.27
Range for cross-corr _{ij}	0.58	0.47	0.25	0.40	0.22	0.37

Table 2. Estimation results from the first simulation

AB, absolute bias; wave AB, weighted average of absolute bias; SD, standard deviation; wave SD, weighted average of standard deviation.

optimization method performed much faster due to the simpler optimization in the second step.

Next, we discuss the differences due to the choice of k. Here we compare the estimates under three models: separable with nugget and nonseparable using the cross-correlation structure (9) with latent dimension k = 1 and k = 2. Since the notion of range is not tied to a specific choice of correlation function, we can compare its estimation under different models. Here we define the effective range as a distance at which the correlation, or cross-correlations, is equal to 0.05. In Table 2 we report results of the simulation study over 400 replicates. For the parameters τ , α , and β we report the absolute bias and standard deviation of estimates. For the parameters μ_i , σ_i , effective range for correlation of variable i for i = 1, ..., p, we report the weighted average of absolute biases and of standard deviations over the index i, where the weights sum to one and are proportional to the true value of the parameter. We do the same for $\|\xi_i - \xi_j\|$ and the effective range for cross-correlations between variables i and j for i, j = 1, ..., p. Nonseparable models gave much better estimates for all parameters, especially, for variances, nugget and effective ranges for cross-correlations. The nonseparable model with k = 2 produces slightly better estimates than the one with k = 1 at the expense of three extra parameters. According to the likelihood ratio test, the model with k = 2 is preferred to the model with k = 1 in 22% of the generated samples.

In the second simulation study, we compare our model with the linear model of coregionalization. To demonstrate the extra flexibility that our model provides, we fit our model and a coregionalization model, when in fact, our model is true. In this regard, we generate samples from a zero-mean two-dimensional spatial Gaussian random field $\{Z_1(s), Z_2(s)\}$ having an underlying covariance specification $\operatorname{cov}\{Z_i(s_1), Z_j(s_2)\}$ based on (7):

$$C_{ij}(\|h\|) = C(\|h\|, \delta_{ij}) = \begin{cases} a_{11}^2 \exp(-\alpha_1 \|h\|) & (i = j = 1), \\ a_{21}^2 \exp(-\alpha_1 \|h\|) + a_{22}^2 \exp(-\alpha_2 \|h\|) & (i = j = 2), \\ \frac{a_{11}a_{21}}{\delta_{12} + 1} \exp\left\{-\frac{\alpha_1 \|h\|}{(\delta_{12} + 1)^{\beta/2}}\right\} & (i \neq j), \end{cases}$$

where $h = s_1 - s_2$. A coregionalization model is a special case of the above specification when $\delta_{12} = \beta = 0$. We set $a_{11} = 1.25$, $a_{21} = 0.75$, $a_{22} = 0.5$, $\alpha_1 = 1$, $\alpha_2 = 3$, $\delta_{12} = 2$ and $\beta = 1$. We generated n = 200 points whose spatial locations were selected at random from the $[0, 20] \times [0, 20]$ square. In Table 3 we report estimation results of 400 simulations. Maximum likelihood

		Proposed model			Linear model of coregionalization		
Parameter	True	2.5%	50.0%	97.5%	2.5%	50.0%	97.5%
μ_1	0	-0.30	0.00	0.31	-0.30	0.00	0.31
μ_2	0	-0.19	0.00	0.20	-0.20	0.00	0.20
a_{11}	1.25	1.08	1.23	1.38	1.08	1.23	1.38
<i>a</i> ₂₁	0.75	0.24	0.69	0.90	0.07	0.21	0.35
<i>a</i> ₂₂	0.50	0.21	0.54	0.83	0.76	0.86	0.95
α_1	1.00	0.73	1.05	1.46	0.71	1.04	1.48
α_2	3.00	0.82	2.82	7.06	1.10	1.59	2.53
β	1.00	0.10	1.00	1.00	_	_	_
δ_{12}	2.00	0.25	2.00	4.60	_	_	_
Cross-corr for $h = 0$	0.28	0.11	0.27	0.40	0.09	0.24	0.37
Range for Z_1	3.22	2.09	3.11	4.50	2.09	3.07	4.66
Range for Z_2	2.42	1.41	2.23	3.21	1.25	1.92	2.72
Range for cross-corr	2.97	0.85	2.53	3.71	0.45	1.48	2.48

lable 3. Estimation results from the second simulation	on
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generates quite reasonable estimates for the proposed model. There is a slight bias in estimating a_{2i} , α_2 and consequently in the range for cross-correlation. The model of coregionalization underestimates the cross-correlation and results in a biased estimate of the range for cross-correlation where the true value lies outside the 95% confidence interval. The table suggests that the model of coregionalization is not flexible enough to provide unbiased estimates for the range and cross-correlation even for the simple setting of just two correlated processes.

5. Application to pollution data from California

We illustrate our modelling approach with a pollution dataset obtained from a collection of monitoring stations in California. The data, which were used by Schmidt & Gelfand (2003) and Majumdar & Gelfand (2007), were obtained from the California Air Resources Board. These authors considered the daily average of carbon monoxide, CO, nitrous oxide, NO, and nitrogen dioxide, NO₂, based on hourly measurements on July 6, 1999.

The locations of 68 monitoring stations were recorded on a degree latitude by degree longitude scale, and five locations were taken out for verification purposes. We took advantage of the fact that in the sampling area, 1° of latitude ≈ 65 km while 1° of longitude ≈ 110 km to calculate the distances between the sites; see Banerjee (2005) for discussion on the effect of distance computations in spatial modelling. Following Schmidt & Gelfand (2003) and Majumdar & Gelfand (2007), in order to achieve approximate normality, we used the logarithm of the daily average of each of these variables. Similarly to these authors, we fit the model with a constant mean structure. Li et al. (2008) tested the structure of the cross-covariance functions of this dataset and concluded that it was highly variable nonseparable and asymmetric, hence that a linear model of coregionalization was not appropriate. Therefore, the cross-covariance $cov{Z_i(s_1), Z_j(s_2)}$ was chosen to be the most parsimonious asymmetric of Type 2 and spatially anisotropic model:

$$C_{ij}(h) = C(h, v_{ij} - \Gamma_{\xi} h) = \frac{\sigma_i \sigma_j}{\|v_{ij} - \Gamma_{\xi} h\| + 1} \exp\left\{-\frac{\alpha \|h\|}{(\|v_{ij} - \Gamma_{\xi} h\| + 1)^{\beta/2}}\right\},$$

for i, j = 1, ..., 3, where $h = s_1 - s_2$, $v_{ij} = \xi_i - \xi_j$ and Γ_{ξ} is a $k \times 2$ matrix. We assumed that the dimensions are points in a k = 1 dimensional space and we reparameterized $\Gamma_{\xi} = \gamma \omega^{\mathsf{T}}$, where $\gamma \ge 0, \omega$ is a two-dimensional vector such that $\omega^{\mathsf{T}}\omega = 1$. Here $\arctan(\omega_2/\omega_1)$ defines the direction

Parameter	2.5%	Estimate	97.5%	Parameter	2.5%	Estimate	97.5%
μ_1	-1.19	-0.94	-0.67	eta	0.10	1.00	1.00
μ_2	-5.58	-5.26	-4.92	α	0.01	0.02	0.04
μ_3	-4.61	-4.38	-4.15	v_{13}	0.44	0.70	1.38
σ_1	0.50	0.65	0.74	v_{23}	-0.73	-0.36	-0.23
σ_2	0.59	0.75	0.87	γ	0.04	0.06	0.12
σ_3	0.44	0.57	0.66	$\arctan(\omega_2/\omega_1)$	71.45	76.64	80.90

Table 4. Maximum likelihood estimates for the pollution data

of anisotropy/asymmetry and γ defines its extent. We used maximum likelihood as a criterion function because of a relatively small sample size.

Table 4 has the parameter estimates and confidence bands obtained by using 500 parametric bootstrapped samples. Figure 3 depicts the estimated spatial correlations and cross-correlations. The estimated correlation matrix with the associated 95% bootstrapped confidence interval in parentheses for the components of the vector evaluated at the same locations is

$$R = \begin{pmatrix} 1 & 0.49 \ (0.29, \ 0.58) & 0.59 \ (0.35, \ 0.69) \\ 1 & 0.74 \ (0.56, \ 0.82) \\ 1 \end{pmatrix}.$$

The observed correlations between these pollutants were 0.46 for CO and NO, 0.56 for CO and NO₂ and 0.77 for NO and NO₂. Schmidt & Gelfand's (2003) estimates with the use of the linear model of coregionalization were 0.23 for CO and NO, 0.32 for CO and NO₂, and 0.51 for NO and NO₂. As we observed in simulations, the linear model of coregionalization produces biased estimates of the cross-correlation due to its lack of flexibility. Because k = 1, we have $v_{12} = v_{13} - v_{23} = 1.06$. The order of distances in the latent space, $|v_{12}| > |v_{13}| > |v_{23}|$, corresponds to the order of correlations between the components of the trivariate vector of pollutants evaluated at the same location, that is, h = 0: $R_{12} < R_{13} < R_{23}$. However, our model is nonseparable, so the order of cross-correlations may differ for some nonzero spatial lags.

Our goal here is to assess the ability of our simplest model to capture spatial patterns. To perform some validation of the model, we use the five held-out stations, at which we predict the levels of all three pollutants with the conditional means and we compare the predictions with the ones obtained by using the linear model of coregionalization of Schmidt & Gelfand (2003) available only for NO₂, and covariance convolution (Majumdar & Gelfand, 2007). These predictions are displayed in Table 5. In most of the cases, the predictions were improved: 8 out of 15 compared to those of Majumdar & Gelfand (2007) and 4 out of 5 compared to those of Schmidt & Gelfand (2003). Specifically, the average differences between the absolute prediction errors for our model and those of Majumdar & Gelfand (2007) were -0.02 for CO, a 4% improvement; -0.63 for NO, a 47% improvement; and -0.04 for NO₂, a 17% improvement. Compared to Schmidt & Gelfand (2003), the improvement was -0.06, that is, 23%. The percentage of improvement is measured as the average, over the five sites, of the difference between the absolute prediction errors for the alternative model and our model, divided by the average, over the five sites, of the absolute prediction error for the alternative model. Predictions based on our model were closer to the held-out values for the difficult-to-predict cases. For instance, for NO, sites 1 and 2, the absolute error was reduced by 45% and 63%, respectively.



Fig. 3. Estimated spatial correlations and cross-correlations at contour levels $0.1, \ldots, 0.5$ for the pollution data.

Site	True	AG Pred	MG Pred	SG Pred	AG vs MG	AG vs SG		
			Prediction of	f CO				
1	-0.89	-0.59	-0.90	_	0.29	_		
2	-0.80	-1.05	-0.95	_	0.10	_		
3	-0.98	-1.10	-0.93	_	0.06	_		
4	-1.67	-1.42	-0.91	_	-0.51	_		
5	-2.30	-0.96	-0.93	_	-0.03	_		
			Prediction of	f NO				
1	-6.50	-4.94	-3.65	_	-1.29	_		
2	-6.50	-5.46	-3.65	_	-1.81	_		
3	-5.45	-5.28	-5.34	_	0.06	_		
4	-4.75	-5.22	-5.34	_	-0.12	_		
5	-5.52	-5.28	-5.32	_	0.04	_		
Prediction of NO ₂								
1	-4.91	-4.33	-4.42	-4.17	0.09	-0.16		
2	-4.34	-4.54	-4.45	-4.58	0.09	-0.04		
3	-4.59	-4.48	-4.44	-4.59	-0.04	0.11		
4	-4.10	-4.20	-4.45	-3.96	-0.24	-0.03		
5	-4.34	-4.34	-4.43	-4.51	-0.08	-0.16		

Table 5. Prediction at five held-out stations for the pollution data

AG Pred, the predictions based on our model; MG Pred, the predictions from Majumdar & Gelfand (2007); SG Pred, the predictions from Schmidt & Gelfand (2003); AG vs MG, difference between absolute prediction error of our model and of Majumdar & Gelfand (2007); AG vs SG, difference between absolute prediction error of our model and of Schmidt & Gelfand (2003).

6. DISCUSSION

We have proposed a new flexible class of cross-covariance functions for multivariate random field modelling and we have described extensions of our models to accommodate the lack of symmetry and lack of variable isotropy. Standard approaches can be used to relax the assumption of spatial isotropy; see, for example, Mateu et al. (2008) and references therein. The choice of cross-covariance models with specific properties can be guided by the outcome of testing procedures proposed by Li et al. (2007, 2008).

An appealing feature of our construction is that existing univariate models of covariance functions can be used due to our approach being based on latent dimensions. Thus, the statistician's toolkit for modelling multivariate random fields is extended in a rather straightforward manner.

One possible weakness of our approach is that if the number p of variables is large, then the integer number $1 \le k \le p$ of latent dimensions could become large too. However, similarly to multi-dimensional scaling, we can reduce the number of parameters in our cross-covariance models by reducing the dimension of the latent space. In our experience, small values of k are usually sufficient. For example, on the pollution data, we obtained better performances than other competing methods already with k = 1.

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APPENDIX

Proof of Proposition 1

To prove that (2) is a covariance function, we use a result similar to Gneiting (2002, p. 599).

LEMMA A1. A continuous, bounded and integrable function C(h, u, v), defined on \mathbb{R}^{d+l+k} , is a covariance function if and only if

$$C_{\omega}(u, v) = \int \exp(-\iota h^{\mathsf{T}}\omega)C(h, u, v)dh, \quad u \in \mathbb{R}^{l}, v \in \mathbb{R}^{k}$$

is a covariance function for almost all $\omega \in \mathbb{R}^d$.

Recall that from Bernstein's theorem (Feller, 1966, p. 439), a completely monotone function $\varphi(t)$ (t > 0), can be represented by

$$\varphi(t) = \int_{(0,\infty)} \exp(-rt) dF(r),$$

where F is nondecreasing. Hence, for (2), we have

$$\begin{split} C_{\omega}(u,v) &= \int \exp(-\iota h^{\mathrm{T}}\omega) \frac{\sigma^2}{\left[\psi_1\left\{\frac{\|u\|^2}{\psi_2(\|v\|^2)}\right\}\right]^{d/2} \{\psi_2(\|v\|^2)\}^{l/2}} \varphi_1\left[\frac{\|h\|^2}{\psi_1\left\{\frac{\|u\|^2}{\psi_2(\|v\|^2)}\right\}}\right] dh \\ &= \sigma^2 \pi^{d/2} \frac{1}{\{\psi_2(\|v\|^2)\}^{l/2}} \int_{(0,\infty)} \exp\left[-\frac{\|\omega\|}{4r} \psi_1\left\{\frac{\|u\|^2}{\psi_2(\|v\|^2)}\right\}\right] \frac{1}{r^{d/2}} dF(r). \end{split}$$

Let $t = ||u||^2/\psi_2(||v||^2)$. Then, similarly to Gneiting (2002), one can show that

$$\varphi_{\omega}(t) = \int_{(0,\infty)} \exp\left\{-\frac{\|\omega\|}{4r}\psi_1(t)\right\} \frac{1}{r^{d/2}} dF(r)$$

is a completely monotone function for any $\omega \in \mathbb{R}^d$. Therefore,

$$C_{\omega}(u,v) = \sigma^2 \pi^{d/2} \frac{1}{\{\psi_2(\|v\|^2)\}^{l/2}} \varphi_{\omega} \left\{ \frac{\|u\|^2}{\psi_2(\|v\|^2)} \right\}, \quad u \in \mathbb{R}^l, v \in \mathbb{R}^k,$$

which is a valid covariance function for any $\omega \in \mathbb{R}^d$ according to Theorem 2 from Gneiting (2002).

Proof of Proposition 2

First, the product $C_{i_1}(h, u, 0)C_{i_2}(h, 0, v)$ is a valid covariance function on \mathbb{R}^{d+l+k} because

$$C_{i_1i_2,\omega}(h,v) = \int \exp(-\iota u^{\mathsf{T}}\omega)C_{i_1}(h,u,0)C_{i_2}(h,0,v)du = C_{i_1,\omega}(h,0)C_{i_2}(h,0,v)$$

is a valid covariance function for almost all $\omega \in \mathbb{R}^l$ since

$$\tilde{C}_{\omega_{i_1},\omega_{i_2}}(h) = \int \exp(-\iota v^{\mathsf{T}} \omega_{i_2}) C_{i_1,\omega_{i_1}}(h,0) C_{i_2}(h,0,v) dv = C_{i_1,\omega_{i_1}}(h,0) C_{i_2,\omega_{i_2}}(h,0)$$

is a valid covariance function for almost all $\omega_{i_1}, \omega_{i_2} \in \mathbb{R}^l$. Hence

$$C_{i_1i_2,\omega}(u,v) = \int \exp(-\iota h^{\mathsf{T}}\omega)C_{i_1}(h,u,0)C_{i_2}(h,0,v)dh$$

is a valid covariance function as well. Therefore, $C_{i_1}(h, u, 0)C_{i_2}(h, 0, v)C_{i_3}(0, u, v)$ is positive definite because

$$C_{i_1i_2i_3,\omega}(u,v) = \int \exp(-\iota h^{\mathsf{T}}\omega)C_{i_1}(h,u,0)C_{i_2}(h,0,v)C_{i_3}(0,u,v)dh = C_{i_1i_2,\omega}(u,v)C_{i_3}(0,u,v)$$

is positive definite. It follows that the product defined by (3) is also positive definite.

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