Spatiotemporal Covariance Functions from Physical Models

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ABSTRACT

Spatiotemporal geostatistics provides tools for coping with the variability and uncertainties encountered in the study of real-world systems. Among these tools, the covariance functions allow us to understand space-time variations in natural processes. Physical models, such as differential equations and physical laws, provide a powerful framework for the generation of covariance functions, and considerably enrich the class of widely used simple covariance functions. This work reviews the category of non-separable covariances generated from physical models, some of which have appeared in the recent geostatistics literature. Visual representations are used to exhibit characteristic features of covariance functions, and methods for developing physically based covariance functions that can cover user-specific needs for a wealth of applications, are presented.

1. INTRODUCTION

The issues of variability and uncertainty are often encountered in the study of natural processes. These may arise from reasons inherent in the dynamics of the process (ontologic causes). Otherwise, the may be due to lack of accurate knowledge regarding the process, in which case we refer to epistemic limitations. This problem is most commonly dealt with by means of statistics. Whereas classical statistics has traditionally displayed shortcomings in the sufficient description of the randomness in natural processes, the Spatiotemporal Random Field (S/TRF) theory (Christakos, 1991; 1992) has offered a powerful framework for this purpose.

Of primary role in the S/TRF theory is the S/TRF $X(\boldsymbol{p})$, where $\boldsymbol{p} = (\boldsymbol{s}, t) \in R^n \times T$ is a composite vector that combines the location vector $\boldsymbol{s}$ in the n-dimensional Euclidean space R^n and the scalar time t along the time axis T. Covariances are functions used in the S/TRF theory that express the behavior of correlations and interdependencies between points in space/time (S/T). Very often, covariances are considered to be functions of only S/T distances between pairs of points $\boldsymbol{p} = (\boldsymbol{s}, t)$ and $\boldsymbol{p}' = (\boldsymbol{s}', t')$, i.e., $\boldsymbol{r} = \boldsymbol{s}' - \boldsymbol{s}$ (indicating spatial homogeneit y) and $\tau = t' - t$ (showing time stationarity). The above are features of the ordinary (or centered) covariances that we will denote by $c_x(\boldsymbol{r}, \tau)$. If it the condition $c_x(\boldsymbol{r}, \tau) = c_x(r = |\boldsymbol{r}|, \tau)$ holds, where $|\boldsymbol{r}|$ is the magnitude of the vector $\boldsymbol{r}$, the field is spatially isotropic in the weak sense.

Any function that is a permissible covariance model (see following section) can be used in the study of natural processes. There exists a variety of S/T separable models (e.g., Christakos and Hristopulos, 1998; Kyriakidis and Journel, 1999), as well as non-separable models in which the space and time components are integrated in the covariance expression (e.g., Christakos 1991, 1992, 2000; Christakos and Hristopulos, 1998; Mardia *et al.*, 1998; Cressie and Huang, 1999; Ma, 2002, 2003a, 2003b; Gneiting, 2002).

This work focuses on the more realistic non-separable covariance functions, and specifically ones based on physical models. The concept of accounting for the underlying physics in a stochastic problem has been successfully tested in Kolovos *et al.*, 2002. Covariance functions built from physical models (when possible) account for the interdependencies in random fields more reliably than *ad hoc* geostatistical models, since physical models incorporate the underlying physics of natural processes. In that sense, physics-based covariance functions have an advantage over commonly used simple models (e.g., the linear or the exponential models). In the following, we will present and visualize some theoretical, physics-based, non-separable covariance models, as well as ways to construct new ones by means of space transformation (STF) operators.

2. PERMISSIBILITY AND SPACE TRANSFORMATIONS OF COVARIANCES

Not all functions are permissible covariance models. Based on Bochner's theorem (Christakos, 1992), a function $c_{x,n}(\boldsymbol{r},t)$ in the $R^n \times T$ domain ($n = 1,2,3$) is in general a permissible ordinary covariance if and only if its spectral density (i.e., its Fourier transform)

$$\tilde{c}_{x,n}(\boldsymbol{k},w) = \int\int d\boldsymbol{r}\,dt\, e^{-i(\boldsymbol{k}\boldsymbol{r}+wt)} c_{x,n}(\boldsymbol{r},t) \qquad (1)$$

is non-negative and its total variation is bounded. Appropriately modified criteria define the permissibility of non-centered covariances (e.g., earlier reference).

New covariance functions can be constructed from permissible ones. In particular, Christakos (1984b, 1986) introduced STF operators that permit constructing covariance functions in two and three dimensions from one-dimensional models. One STF operator links a covariance model $c_{x,1}$, in $R^1 \times T$, with covariance models $c_{x,n}$, in $R^n \times T$ $(n = 2, 3)$, by means of the integral relation

$$c_{x,n}(r,t) = E_n \int_0^1 du\,(1-u^2)^{(n-1)/2} c_{x,1}(ur,t), \qquad (2)$$

where $E_n = 2\Gamma(n) \big/ \left(\sqrt{\pi}\,\Gamma[(n-1)/2]\right)$ and Γ is the gamma function. The STF analysis implies that from a permissible covariance model in $R^1 \times T$, a new model can be derived in $R^n \times T$ by means of Eq. (2).

Another STF operator relates the spectral density $\tilde{c}_{x,1}$ (in $R^1 \times T$) with the spectral densities $\tilde{c}_{x,n}$ (in $R^n \times T$; $n = 2, 3$) by means of the following equations:

$$\tilde{c}_{x,2}(k,w) = = \int_k^\infty du (u^2 - k^2)^{1/2} \tfrac{d}{du}[u^{-1} \tfrac{d}{du} \tilde{c}_{x,1}(u,w)] \qquad (3a)$$

$$\tilde{c}_{x,3}(k,w) = -(1/2\pi) k^{-1} \tfrac{d}{dk} \tilde{c}_{x,1}(k,w) \qquad (3b)$$

Expressions analogous to Eqs. (2) and (3) in $R^n \times T$ can be derived from different STF operators.

A permissible covariance model c_x in $R^1 \times T$ is not necessarily permissible in $R^n \times T$. One needs to derive the spectral density $\tilde{c}_{x,n}$, and then test if it satisfies the requirements of Bochner's theorem.

In contrast, any model that is permissible in n dimensions is also permissible in n' dimensions, where $n' < n$ (Christakos, 1984a). In some cases it may be more convenient mathematically to investigate the permissibility of a covariance model in $R^3 \times T$, regardless of the domain of interest.

3. COVARIANCES GENERATED FROM PHYSICAL MODELS

We will classify the covariances in this category based on the method by which they are generated Many of them are derived from solutions of partial differential equations (PDE). Others are based on a variety of physical models, as demonstrated in the following.

3.1 Models derived from differential equations

A large class of non-separable spatiotemporal covariance models is associated with the general stochastic PDE $\partial/\partial t[X(\boldsymbol{p})] = \mathrm{L}_s[X(\boldsymbol{p})]$, where L_s is a linear spatial differential operator in R^n. An example from this class is the general form of (non-centered) covariances given below (Christakos and Hristopulos, 1998)

$$C_x(\boldsymbol{s},t;\boldsymbol{s}',t') = \\ = \sum_{j,k=0}^{\infty} c_{jk}\, c_{1j}(\boldsymbol{s})c_{1k}(\boldsymbol{s}')c_{2j}(t)c_{2k}(t') \quad (4)$$

where c_{1j} and c_{2j} represent eigenfunctions (modes) of the PDE. Each mode has an amplitude A_j, which is determined from the boundary and initial conditions (B/IC). In Eq. (4) the coefficients c_{jk} represent correlations of the mode coefficients, i.e., the ensemble average $c_{jk} = \overline{A_j A_k}$. Randomness in the covariance model of Eq. (4) can be introduced, respectively, by: (*i*) the B/IC, leading to random coefficients A_j; (*ii*) the differential operator L_s leading to random eigenfunctions c_{1j}; and (*iii*) by both of the above. Models (4) may be non-homogeneous / non-stationary due to a number of reasons, including the B/IC effects.

For visualization purposes, we followed the example discussed in Christakos and Hristopulos (1998) in $R^1 \times T$. A diffusion PDE is considered with a parabolic initial concentration profile given by $f(s) = c_0 4(s/L)(1-s/L)^{-1}$, where c_0 is a random variable with $\overline{c_0^2} = 1$ and L is the domain size. Then $c_{jk} = a_j a_k$, $c_{1j} = \cos(j\pi s/L)$ and $c_{2j} = \exp(-D j^2 \pi^2 t/L^2)$, where D is the diffusion coefficient; also, $a_j = -8(j\pi)^{-2} - [1+(-1)^j]$ (if $j > 0$), and $a_j = 2/3$ (if $j = 0$). By inserting these parameters in Eq. (4) and letting $L = 1$ we obtained the covariance $C_x(s,t;s',t')$ plotted in Figure 1.

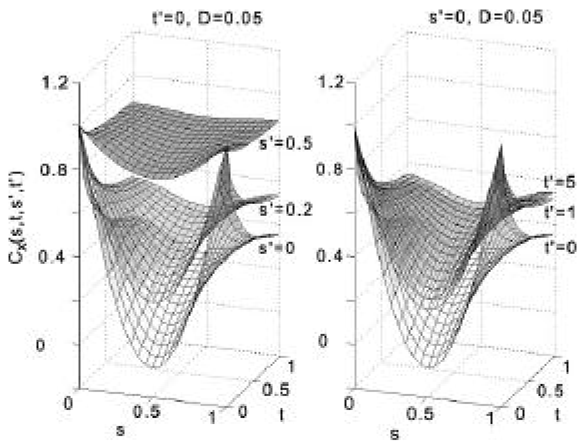

Figure 1: Plots of the non-separable covariance model of Eq. (4) for a spatial domain of size $L = 1$ in the $R^1 \times T$ domain. The diffusion coefficient is D=0.05.

This function depends on the S/T coordinates of both points $p = (s,t)$ and $p' = (s',t')$, and not just on the space and time distances between the points. In Figure 1 we plot the covariance values between points in the (s,t)-domain, and the points $(s'=0, t')$ and $(s', t'=0)$ throughout the length L for D=0.05.

The following covariance model

$$c_x(r,t) = \\ = 0.5[\exp(-ar)Erfc(a\sqrt{c^{-1}t} - 0.5r\sqrt{ct^{-1}}) \\ + \exp(ar)Erfc(a\sqrt{c^{-1}t} + 0.5r\sqrt{ct^{-1}})] \quad (5)$$

is based on a parabolic PDE model initially proposed by Heine (1955). The a and c are coefficients associated with the parabolic PDE, and $Erfc(x)$ is the complementary error function defined as:

$$Erfc(x) = \begin{cases} (2/\sqrt{\pi})\int_x^{\infty} dv \exp(-v^2), & \text{if } x \geq 0 \\ 2 - Erfc(-x), & \text{if } x < 0 \end{cases}$$

Model (5) represents spatially homogeneous and temporally stationary fields in $R^1 \times T$. Notice that $c_x \to 2Erfc(a\sqrt{t/c})$ as $r \to 0$; and

$c_x \to s^2$ as $r, t \to 0$. The model (5) is plotted in Figure 2A for a choice of a- and c-values in $R^1 \times T$. The values of the parameters affect the ranges and shape of the covariance models.

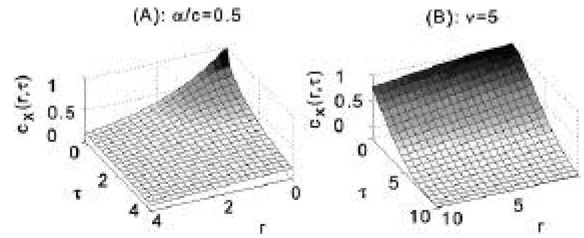

Figure 2: (A) Plot of the non-separable covariance model of Eq. (5) in the $R^1 \times T$ domain for the ratio value a/c=0.5. (B) Plot of the non-separable covariance model of Eq. (8) in the $R^2 \times T$ domain for the parameter values of a =0.5 and v=5.

The covariance, e.g., decreases faster for increasing values of the a/c ratio. Using Eq. (3), it is found that Heine's model (5) is permissible for $n=2$ and 3, as well. Certain extensions of the model (5) were proposed by Ma (2003b). Furthermore, new covariance models in $R^n \times T$ $(n>1)$ are derived from model (5) by applying the space transform of Eq. (2), i.e.,

$$c_{x,n}(r,t) = 0.5E \int_0^1 du\,(1-u^2)^{(n-1)/2} \times$$
$$\times [\exp(-aur)\, Erfc(a\sqrt{c^{-1}t} - 0.5ur\sqrt{ct^{-1}}) +$$
$$+ \exp(aur) Erfc(a\sqrt{c^{-1}t} + 0.5ur\sqrt{ct^{-1}})] \quad (6)$$

General PDE can generate new classes of permissible spatiotemporal covariance functions based on other well-known functions. For example, Christakos (1992) used in $R^2 \times T$ the physical PDE $D_{s,t} Z(s,t) = X(s,t)$, where $s = (s_1, s_2)$ and $D_{s,t} = -a\,\partial^2/\partial t^2 + b(\partial^4/\partial s_1^4 + \partial^4/\partial s_2^4) + 2b\,\partial^4/\partial s_1^2 \partial s_2^2$ to derive new spatiotemporal covariances $c_z(\boldsymbol{r}, t)$ starting from existing ones, $c_x(\boldsymbol{r}, t)$, as follows

$$c_z(\mathbf{r},t) = \int\int d\mathbf{k}\, dw\, e^{i(\mathbf{k}\cdot\mathbf{r}+wt)} \frac{\tilde{c}_x(\mathbf{k},w)}{(bk^4 + aw^2)^2} \quad (7)$$

where $\boldsymbol{r} = (r_1, r_2)$, $\boldsymbol{k} = (k_1, k_2)$, a and b are positive coefficients, and $\tilde{c}_x(\boldsymbol{k}, w)$ is the spectral density of $c_x(\boldsymbol{r}, t)$. For illustration, we let $a = b = 1$ and use a spectral density of the form $\tilde{c}_x(\boldsymbol{k}, w) = 2\pi\,\delta(w - \boldsymbol{k}\cdot\boldsymbol{v})\exp(-\alpha^2 \boldsymbol{k}^2/4)$, where $\boldsymbol{v}$ is a known velocity vector. Then, assuming spatial isotropy, Eq. (7) yields

$$c_z(\mathbf{r},t) = 0.5a \int_0^\infty dk\, k^{-3}(k^2 + v^2)^{-2} \times \exp(-\alpha^2 k^2/4)\, J_0[k(r + vt)] \quad (8)$$

in $R^2 \times T$, where $v = |\boldsymbol{v}|$. Eq. (8) is calculated numerically leading to the covariance plot of Figure 2B.

Similarly, starting from the physical PDE $L_{\boldsymbol{p}}[Z(\boldsymbol{p})] = X(\boldsymbol{p})$ in $R^n \times T$, where $L_{\boldsymbol{p}} = (\partial/\partial t) L_{\boldsymbol{s}}$, S/T covariance models can be generated by means of the equation

$$c_z(\boldsymbol{p}, \boldsymbol{p}') = \int\int d\boldsymbol{u}\, d\boldsymbol{u}'\, c_x(\boldsymbol{u}, \boldsymbol{u}')\, g(\boldsymbol{p}, \boldsymbol{u})\, g(\boldsymbol{p}', \boldsymbol{u}'),$$

where g is the Green's function that obeys the equation $L_{\boldsymbol{p}}[g(\boldsymbol{p}, \boldsymbol{u})] = \delta(\boldsymbol{p} - \boldsymbol{u})$. This process produces a versatile class of non-separable covariance models, not plotted here.

3.2 Models generated from physical rules

The diffusion equation inspired a non-separable spatiotemporal covariance model in $R^n \times T$ $(n = 1, 2, 3)$ (e.g., Christakos, 2000):

$$c_x(r,t) \cong (4a\pi t)^{-n/2} \exp(-r^2/4a\,t) \quad (9)$$

where $a > 0$. Note that this model tends to a delta function as $t \to 0$. The symbol "$\cong$" denotes that the covariance follows this functional form asymptotically but not close to the origin. To obtain permissible covariance models, the singularity at zero lag must be tamed, e.g., by means of a short-range cutoff. Short-range cutoffs can be introduced in relation to physical scales of the underlying process

(Hristopoulos, 2002). The covariance model (9) is plotted for $\alpha = 0.5$ in $R^3 \times T$ (n=3) in Figure 3A.

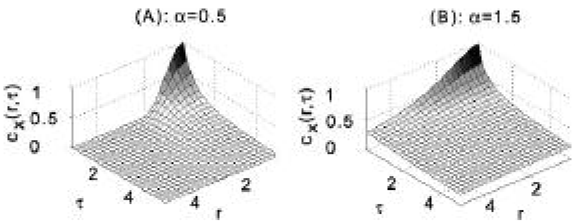

Figure 3: (A) Plot of the non-separable covariance model of Eq. (9) in the $R^3 \times T$ domain. (B) Plot of the model (11b), again in $R^3 \times T$, for selected values of the parameter α.

Clearly, the shape of the covariance, the correlation ranges and the behavior near the space-time origin depend on the n- and α-parameter values.

Furthermore, starting from Eq. (9) with $n = 1$ and using Eq. (2), new covariance models can be found in $R^n \times T$ ($n = 2, 3$) as follows

$$c_{x,n}(r,t) = B_n \int_0^1 du\,(1-u^2)^{(n-1)/2} \times \exp(-ur^2/4\alpha t) \qquad (10)$$

where $B_n = (4\alpha\pi t)^{-1/2} E_n$. Since any model that is permissible in n dimensions is also permissible in $n' < n$ dimensions, in $R^2 \times T$ Eq. (9) leads to the covariance model

$$c_{x,2}(r,t) = 0.125\pi^{1/2}(\alpha t)^{-1/2} E_2 \times KummerM[0.5,\, 2, -Z_A] \qquad (11a)$$

where $Z_A = r^2(4\alpha t)^{-1}$, $t > 0$, and the $KummerM(\cdot)$ function is a solution to the Kummer's differential equation (Abramowitz and Stegun, 1972). In $R^3 \times T$, Eq. (9) yields the model(with $r,\, t > 0$):

$$c_{x,3}(r,t) = 0.5 r^{-1} E_3 [(1 - 0.5 Z_A^{-1}) Erf(Z_A^{1/2}) + (\pi Z_A)^{-1/2} \exp(-Z_A)] \qquad (11b)$$

Eq. (11b) is plotted in Figure 3B for $\alpha = 1.5$.

Different formulations and extensions of Eq. (9) are possible (in order to deal with the singularity at zero, to account for physical features of the underlying process etc.). Gneiting (2002) proposes space-time formulations which involve the addition of constants after the time lag. A similar approach was suggested by Hristopulos (2002). In this way Eq. (9) may be modified, e.g., as follows

$$c_x(r,t) = (\beta t^{2\gamma} + 1)^{-n/2} \exp[-r^2/(\beta t^{2\gamma} + 1)] \qquad (12a)$$

($0 \le \beta \le 1$, $0 < \gamma \le 1$). The covariance class of Eq. (12a) has been used in fluid mechanics studies (e.g., Monin and Yaglom, 1975). Certain generalizations of the form

$$c_x(r,t) = (B/(t-\zeta)^{\lambda}) f(r^2/c(t-\zeta))$$

have also been studied, where B, ζ, c, and λ are physical coefficients and $f(\cdot)$ is a suitable function (see, Monin and Yaglom, 1975). Starting from Eq. (12a) with $n = 1$, $\gamma = 0.5$, and applying the STF of Eq. (2) we find the new covariance models

$$c_{x,2}(r,t) = 0.25\pi(\beta t + 1)^{-1/2} \times E_2\, KummerM[0.5, 2, -Z_B] \qquad (12b)$$

and

$$c_{x,3}(r,t) = 0.5\pi^{1/2} r^{-1} E_3 [(1 - 0.5 Z_B^{-1}) \times Erf(Z_B^{1/2}) + (\pi Z_B)^{-1/2} \exp(-Z_B)] \qquad (12c)$$

where $Z_B = r^2(\beta t + 1)^{-1}$. Model (12c) is plotted in Figure 4A for a selected value of the parameter β. Atmospheric turbulence studies (e.g., Pope, 2000) lead to further extensions of the covariance class of Eq. (9) in the form of $c_x(r,t) \cong (\beta t)^{-\mu} \exp(-r^2/\alpha t)$, which includes the cases $\mu = 0$ and $\mu > 1.5$ in $R^3 \times T$ (the coefficients μ, α and β obtain physical meaning in the context of the turbulence study considered).

Moreover, based on physical considerations a series of spatiotemporal covariance models can be derived from Eq. (9), such as

$$c_x(r,t) = (1+bt^2)^{-3/2}[1-0.5r^2 \times (1+bt^2)^{-1}]\exp[-0.5r^2/(1+bt^2)] \quad (13a)$$

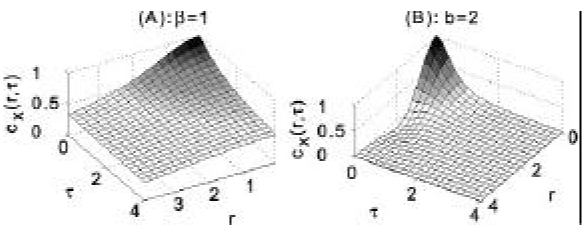

Figure 4: (A) Plot of the non-separable covariance model (12c) in $R^3 \times T$ for the parameter value $b=1$. (B) Plot of the non-separable covariance model of Eq. (13b) in $R^2 \times T$ for the parameter value $b=2$.

and

$$c_x(r,t) = (1+bt^2)^{-5/2} \times \{1-r^2(1+bt^2)^{-1}+r^4[8(1+bt^2)^2]^{-1}\} \times \exp[-0.5r^2/(1+bt^2)] \quad (13b)$$

Covariance model (13b) in the $R^2 \times T$ domain is plotted in Figure 4B for $b=2$. Among the noticeable features of this plot is the presence of "hole effects", mainly, along the space direction.

4. CONCLUSIONS

In this work permissible, non-separable covariance functions based on physical models were reviewed, and approaches for constructing new models were proposed The suggested models broaden the scope for the researchers who need to employ covariance functions in their studies, and offer model options based in physics and differential equations for investigations of space/time variations in natural systems.

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