STATISTICAL TOOLS IN RENEWABLE ENERGY MODELING: PHYSICAL BASED, NON-SEPARABLE SPATIOTEMPORAL COVARIANCE MODELS

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ABSTRACT

Covariance functions are powerful statistical tools for the understanding and analysis of the variability and uncertainty in natural systems. The category of non-separable spatiotemporal covariances offers advanced options and added flexibility in modeling the joint space/time structure of real-world processes that lie in the heart of renewable energy modeling. This work offers a review of covariances generated from physical models alongside with visual representations for the illustration of their characteristic features. In addition, methods are presented to further develop and expand the collection of such functions.

Key words: Spatiotemporal, renewable energy modeling, stochastic processes, random fields, geostatistics.

1. INTRODUCTION

Renewable energy modeling is one of the vibrant areas for applications of spatiotemporal mapping analysis. Space/time mapping of the incoming solar energy and modeling of the solar cells performance; analysis of materials used to build photovoltaics and their properties; modeling of the wind fields and identification of the optimal locations for wind turbines; estimation of the technical potential of renewable energy. These are but a few instances of space/time-dependent natural processes and measures in the field, which can be studied using spatiotemporal prediction techniques. The estimation of unsampled

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values is tightly related to the subsequent creation of meaningful, informative maps that can be instrumental in pre-testing technical options, projecting research results, analyzing the financial feasibility of potential solutions, providing cost-estimation, and eventually assisting decision-making. In principle, the dynamics of such processes on one hand, and limitations in our accurate knowledge of the phenomena on the other, raise the issues of naturally occurring variability and uncertainty in the studies. This problem is efficiently dealt with by means of the stochastic representation of natural processes, where statistical tools are used to quantify and account for these uncertainties at the modeling stage. A powerful framework in the description and study of stochastic processes is offered by the Spatiotemporal Random Field (S/TRF) theory (Christakos, 1991; 1992).

The S/TRF theory provides understanding of stochastic processes $X(\boldsymbol{p})$, where $\boldsymbol{p}=(\boldsymbol{s},t)\in R^n\times T$, by analyzing their space/time structure, and models their behavior on the basis of the available knowledge bases such as physical laws, epistemic principles, empirical equations, field measurements, hard or soft data. The spatiotemporal structure of $X(\boldsymbol{p})$ examines how points in space and time are correlated, and expresses these interdependencies using statistical concepts; e.g., the first order stochastic moments of the S/TRF represent underlying systemic trends of the field. The second order moments describe fluctuations at a smaller scale, and are also known as covariances.

In particular, covariances express correlations between pairs of points in space/time, $\boldsymbol{p}=(\boldsymbol{s},t)$ and $\boldsymbol{p}'=(\boldsymbol{s}',t')$. Permissible functions can be used to express these correlations. In general, a function is a permissible covariance model if and only if its Fourier transform is non-negative and its total variation is bounded. Two main families of covariances are the ordinary (or centered) covariances and the generalized ones. The first category is usually associated with spatially homogeneous and temporally stationary S/TRF, whereas the second family is used with non-homogeneous/non-stationary S/TRF. Covariances are also categorized as separable or non-separable, depending on whether the covariance function can be decomposed into purely spatial and temporal components or not, respectively.

The present work focuses on the physically more realistic non-separable covariance functions. There exist several theoretical models for such covariances in the spatiotemporal stochastics and geostatistics, as well as in the classical statistics literature. We aim to present ways to create new models of non-separable spatiotemporal covariance functions. We also illustrate some theoretical models of such covariance functions that are based on physical models considerations that may be of particular interest in the renewable energy modeling field.

2. SPACE TRANSFORMATION OPERATORS

Construction of new covariance models is possible, as long as the candidate functions are tested successfully for permissibility. A fruitful method that creates new covariance functions from permissible ones was introduced by Christakos (1984b, 1986). According to the method, space transformation operators (STF) are introduced that permit constructing covariance functions in two and three dimensions from one-dimensional models.

More specifically, in one instance 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

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

where $E_n = 2\Gamma(n) \big/ \left(\sqrt{\pi}\Gamma\left[(n-1)/2\right]\right)$ and Γ is the gamma function.

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:

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

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

The above methods can be further extended, as the area of STF operators is open for reasearch, and consequently similar expressions to the ones in Eqs. (1) and (2) in $R^n \times T$ can be derived from different STF operators.

According to Christakos (1984a), covariance models that are permissible in n dimensions are also permissible in $n' < n$. In that sense, 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 spatial dimensionality of the domain of interest. Note, however, that a permissible covariance model c_x in $R^1 \times T$ is not necessarily permissible in $R^n \times T$. Following the permissibility condition, one needs to derive the spectral density $c_{x,n}$, and then test if it satisfies the requirements of Bochner's theorem.

3. COVARIANCES GENERATED FROM PHYSICAL MODELS

This section focuses on the presentation of ordinary, non-separable spatiotemporal covariances generated by physical models and considerations. Solutions of partial differential equations (PDE) are a common source for such covariance models, as demonstrated in the following.

3.1 Models derived from differential equations

I. The general stochastic PDE $\partial/\partial t[X(\boldsymbol{p})] = L_s[X(\boldsymbol{p})]$ is used for the construction of a large class of non-separable spatiotemporal covariance models. In the PDE expression, L_s is a linear spatial differential operator in R^n. For example, Christakos and Hristopulos (1998) provide the following form of (non-centered) covariances based on the preceding PDE:

$$C_X(\boldsymbol{s},t;\boldsymbol{s}',t') = \begin{cases} \sum_{j,k=0}^{\infty} c_{jk}\,\chi_{1j}(\boldsymbol{s})\,\chi_{1k}(\boldsymbol{s}')\,\chi_{2j}(t)\,\chi_{2k}(t') \\ \sum_{j,k=0}^{\infty} A_j A_k\, c_{\chi(j,k)}(\boldsymbol{s},\boldsymbol{s}')\,\chi_{2j}(t)\chi_{2k}(t') \\ \sum_{j,k=0}^{\infty} \overline{A_j A_k\,\chi_{1j}(\boldsymbol{s})\,\chi_{1k}(\boldsymbol{s}')}\,\chi_{2j}(t)\,\chi_{2k}(t') \end{cases}, \qquad \text{(3a-c)}$$

where χ_{1j} and χ_{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. (3a) the coefficients c_{jk} represent correlations of the mode coefficients, i.e., the ensemble average $c_{jk} = \overline{A_j A_k}$. In Eq. (3b) the function $c_{\chi(j,k)}$ denotes the mode correlation $\overline{\chi_{1j}(\boldsymbol{s})\chi_{1k}(\boldsymbol{s}')}$ and A_j are deterministic mode amplitudes. In Eq. (3c) the A_j are random variables to be determined from the B/IC. Randomness in the covariance model of Eq. (3) can be introduced, respectively, by: (*i*) the B/IC, leading to random coefficients A_j; (*ii*) the differential operator $L_{\boldsymbol{s}}$ leading to random eigenfunctions χ_{1j}; and (*iii*) by both of the above. Models (3) 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 $c_{jk} = a_j\, a_k$, $\chi_{1j} = \cos(j\pi s/L)$ and $\chi_{2j} = \exp(-D\, j^2 \pi^2 t/L^2)$, 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. (3) and letting $L = 1$ we obtained the covariance $C_x(s,t;s',t')$ plotted in Fig. 1. Note that $C_x(s,t;s',t')$ 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 particular, the plots illustrate 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.

II. Heine (1955) proposed a parabolic PDE model, based on which the following covariance model is built:

$$c_x(r,\tau) = 0.5[\exp(-ar)\,Erfc(a\sqrt{c^{-1}\tau} - 0.5r\sqrt{c\,\tau^{-1}}) + \exp(ar)\,Erfc(a\sqrt{c^{-1}\tau} + 0.5r\sqrt{c\,\tau^{-1}})] \quad (4)$$

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 (4) represents spatially homogeneous and temporally stationary fields in $R^1 \times T$. Its form suggests that $c_x \to 2Erfc(a\sqrt{\tau/c})$ as $r \to 0$; and $c_x \to \sigma^2$ as $r, \tau \to 0$. The above model is plotted in Fig. 2A for a selected a/c ratio in $R^1 \times T$. The values of the parameters affect the ranges and shape of the covariance models. The covariance, e.g., decreases faster for increasing values of the a/c ratio. Certain extensions of the model (4) were proposed by Ma (2003b).

Using Eq. (1), it is found that Heine's model (4) is permissible for $n = 2$ and 3, as well. Furthermore, new covariance models in $R^n \times T$ ($n > 1$) are derived from model (4) by applying the space transform of Eq. (2), i.e.,

$$c_{X,n}(r,\tau) = 0.5\,E\int_0^1 du\,(1-u^2)^{(n-1)/2}[\exp(-aur)\,Erfc(a\sqrt{c^{-1}\tau} - 0.5ur\sqrt{c\,\tau^{-1}}) + \exp(aur)\,Erfc(a\sqrt{c^{-1}\tau} + 0.5ur\sqrt{c\,\tau^{-1}})] \quad (5)$$

Fig. 2B displays a plot of model (5) in $R^3 \times T$ for the same ratio α/c =0.5 used in Fig. 2A.

III. 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 $D_{s,t} Z(\boldsymbol{s},t) = X(\boldsymbol{s},t)$, where $\boldsymbol{s} = (s_1, s_2)$ and $D_{\mathbf{s},t} = -a\, \partial^2 / \partial t^2 + b(\partial^4 / \partial s_1^4 + \partial^4 / \partial s_2^4) + 2b\, \partial^4 / \partial s_1^2 \partial s_2^2$ to derive new spatiotemporal covariances $c_z(\boldsymbol{r},\tau)$ starting from existing ones, $c_x(\boldsymbol{r},\tau)$, as follows

$$c_Z(\boldsymbol{r},\tau) = \int\int d\boldsymbol{k}\, dw \exp[i(\boldsymbol{k}\cdot\boldsymbol{r} + w\tau)]\, (b\boldsymbol{k}^4 + a\,w^2)^{-2} \tilde{c}_X(\boldsymbol{k},w) \tag{6}$$

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 $c_x(\boldsymbol{r},\tau)$. 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. (6) yields

$$c_Z(\boldsymbol{r},\tau) = 0.5\alpha \int_0^\infty dk\, k^{-3}(k^2 + v^2)^{-2} \exp(-\alpha^2 \boldsymbol{k}^2/4)\, J_0[k(r + v\,\tau)] \tag{7}$$

in $R^2 \times T$, where $v = \|\boldsymbol{v}\|$. Eq. (7) is calculated numerically leading to the covariance plot of Fig. 2C and 2D, for the combinations of α =0.5 with v =3 and v =5, respectively.

IV. 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

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

$$c_x(r,\tau) \cong (4\alpha\pi\tau)^{-n/2} \exp(-r^2/4\alpha\tau) \tag{8}$$

where $\alpha > 0$. Note that this model tends to a delta function as $\tau \to 0$. 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 are defined with respect to the physical scales of the underlying process and can be introduced either in the real or the frequency space (Hristopoulos, 2002). The covariance model (8) is plotted for $\alpha = 0.5$ in $R^2 \times T$ ($n = 2$, Fig. 3A), and in $R^3 \times T$ ($n = 3$, Fig. 3B). 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. (8) with $n = 1$ and using Eq. (2), new covariance models can be found in $R^n \times T$ ($n = 2, 3$) as follows

$$c_{X,n}(r,\tau) = B_n \int_0^1 du\,(1-u^2)^{(n-1)/2} \exp(-ur^2/4\alpha\tau), \tag{9}$$

where $B_n = (4\alpha\pi\tau)^{-1/2} E_n$. Since any model that is permissible in n dimensions is also permissible in $n' < n$ dimensions, in $R^2 \times T$ Eq. (8) leads to the covariance model

$$c_{X,2}(r,\tau) = 0.125\pi^{1/2}(\alpha\tau)^{-1/2} E_2\, KummerM[0.5, 2, -Z_A] \tag{10a}$$

where $Z_A = r^2(4\alpha\tau)^{-1}$, $\tau > 0$, and the $KummerM(\cdot)$ function is a solution to the Kummer's differential equation (Abramowitz and Stegun, 1972). In $R^3 \times T$, Eq. (8) yields the model (with $r, \tau > 0$):

$$c_{X,3}(r,\tau) = 0.5 r^{-1} E_3 [(1 - 0.5 Z_A^{-1})\, Erf(Z_A^{1/2}) + (\pi Z_A)^{-1/2} \exp(-Z_A)] \tag{10b}$$

Selecting a value of α = 1.5, Eq. (10a) is plotted in Fig. 3C, and Eq. (10b) is visualized in Fig. 3D.

II. Different formulations and extensions of Eq. (8) are possible. This flexibility allows to account for specific case-related physical features of the underlying process, to deal with the singularity at zero, 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. (8) may be modified, e.g., as follows

$$c_X(r,\tau) = (\beta\,\tau^{2\gamma} + 1)^{-n/2} \exp[-r^2 /(\beta\,\tau^{2\gamma} + 1)] \qquad (11a)$$

($0 \le \beta \le 1,\ 0 < \gamma \le 1$). The covariance class of Eq. (11a) has been used in fluid mechanics studies (e.g., Monin and Yaglom, 1975). Certain generalizations of the form

$$c_X(r,\tau) = (B/(\tau-\zeta)^{\lambda})\,\phi(r^2/\chi(\tau-\zeta))$$

have also been studied, where B, ζ, χ, and λ are physical coefficients and $\phi(\cdot)$ is a suitable function (see, Monin and Yaglom, 1975). Starting from Eq. (11a) with $n=1$, $\gamma = 0.5$, and applying the STF of Eq. (2) we find the new covariance models

$$c_{X,2}(r,\tau) = 0.25\pi(\beta\tau+1)^{-1/2}\, E_2\, KummerM[0.5, 2, -Z_B] \qquad (11b)$$

and

$$c_{X,3}(r,\tau) = 0.5\pi^{1/2} r^{-1} E_3 [(1-0.5 Z_B{}^{-1})\, Erf(Z_B{}^{1/2}) + (\pi\, Z_B)^{-1/2} \exp(-Z_B)] \qquad (11c)$$

where $Z_B = r^2(\beta\tau+1)^{-1}$. Models (11b) and (11c) are plotted in Fig. 4A and 4B, respectively, 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. (8) in the form of $c_X(r,\tau) \cong (b\,\tau)^{-m} \exp(-r^2/\alpha\,\tau)$, which includes the cases $m=0$ and $m>1.5$ in $R^3 \times T$

(the coefficients m, a and b obtain physical meaning in the context of the turbulence study considered).

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

$$c_X(r,\tau) = (1+b\tau^2)^{-3/2}\,[1-0.5r^2(1+b\tau^2)^{-1}]\,\exp[-0.5r^2/(1+b\tau^2)] \qquad (12a)$$

and

$$c_X(r,\tau) = (1+b\tau^2)^{-5/2}\,\{1-r^2(1+b\tau^2)^{-1}+r^4[8(1+b\tau^2)^2]^{-1}\}\,\exp[-0.5r^2/(1+b\tau^2)] \qquad (12b)$$

Models (12a) and (12b) in the $R^2 \times T$ domain are illustrated in Fig. 4C and 4D, respectively, for $b = 2$. Note in these plots the presence of "hole effects", which are mostly evident along the space direction.

4. GENERALIZED COVARIANCES

The S/TRF-ν/μ theory of continuity orders ν in space and μ in time is the main basis for the definition of generalized spatiotemporal covariance functions, which are asociated with non-homogeneous/non-stationary data. We present here a noticeable class of non-separable covariances that is useful for natural processes with white noise residuals, and has been widely used in the the area of applied geostatistics. The class is given by

$$\kappa_X(r,\tau) = \alpha_0\,\delta(r)\delta(\tau) + \delta(r)\sum\nolimits_{\zeta=0}^{\mu} a_\zeta\,(-1)^{\zeta+1}\tau^{2\zeta+1} + \delta(\tau)\sum\nolimits_{\rho=0}^{\nu} b_\rho\,(-1)^{\rho+1} r^{2\rho+1} +$$
$$\sum\nolimits_{\rho=0}^{\nu}\sum\nolimits_{\zeta=0}^{\mu} d_{\rho/\zeta}\,(-1)^{\rho+\zeta} r^{2\rho+1}\tau^{2\zeta+1} + \delta_{n,2}\,r^{2\nu}\log r\sum\nolimits_{\zeta=0}^{\mu}(-1)^{\zeta} c_\zeta\,\tau^{2\zeta+1} \qquad (13)$$

where $\delta(r)$ and $\delta(\tau)$ represent the spatial and temporal delta functions, respectively, $\delta_{n,2}$ is Kronecker's delta, and coefficients α_0, a_ζ, b_ρ c_ζ, $d_{\rho/\zeta}$ are defined in a suitable manner. The first three terms in Eq. (13) represent discontinuities at the space-time origin; the fourth term is purely polynomial; the fifth term, which is logarithmic in the space lag, is obtained only in $R^2 \times T$. A representation of the general model (13) is plotted in Fig. 5, where we assumed that $\alpha_0 = a_\xi = b_\rho = c_\xi = 0$, $d_{0/0} = d_{2/1} = 1/4$, $d_{0/1} = 1/16$, $d_{1/0} = 1/2$, $d_{1/1} = 1/8$, and $d_{2/0} = 1$.

4. DISCUSSION

This work reviews spatiotemporal, physically-based, non-separable covariance functions that have been developed in the geostatistics community in the last two decades. It also presents methods that enable the expansion and construction of new covariance models, whereas additional models can be constructed by the linear superposition of permissible ones. This enhanced collection of tools serves the accurate representation of the spatiotemporal continuity and variability in natural processes, and is invaluable for the tasks of spatiotemporal prediction in the developing field of renewable energy modeling. These tools are based on solid theoretical foundations; many of those have been successfully tested in a variety of interdisciplinary areas of research (e.g., geostatistics, risk analysis, atmospheric physics, etc.); finally, they offer increased flexibility and further development prospects to allow a precise shaping of their characteristics to the area-specific, emerging needs of modeling in the renewable energy domain.

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Figures

Figure 1: Plots of the non-separable covariance model of Eq. (3) for a spatial domain of size L =1 in the $R^1 \times T$ domain. The diffusion coefficient is D =0.05.

Figure 2: (A) Plot of the non-separable covariance model of Eq. (4) in the $R^1 \times T$ domain and (B) in the $R^3 \times T$ domain, for the ratio value α / c =0.5. In the lower pane, plots of the non-separable covariance model of Eq. (7) in the $R^2 \times T$ domain for the parameter values of α =0.5 and v=3 (C) and v=5 (D).

Figure 3: Plots of the non-separable covariance model of Eq. (8) in the $R^2 \times T$ domain (plot A), in the $R^3 \times T$ domain (plot B), of the model (10a) (plot C) and of the model (10b) (plot D) for selected values of the parameter α.

Figure 4: The top row shows plots of the non-separable covariance model of Eq. (11b) (plot A) and of the model (11c) (plot B) for selected values of the parameter b. In the bottom row, plots of the non-separable covariance models of Eq. (12a) (plot C) and of Eq. (12b) (plot D) for the parameter value $b = 2$.

Figure 5: Plot of a non-separable generalized covariance in the $R^2 \times T$ domain based on model (13).

Figure 1

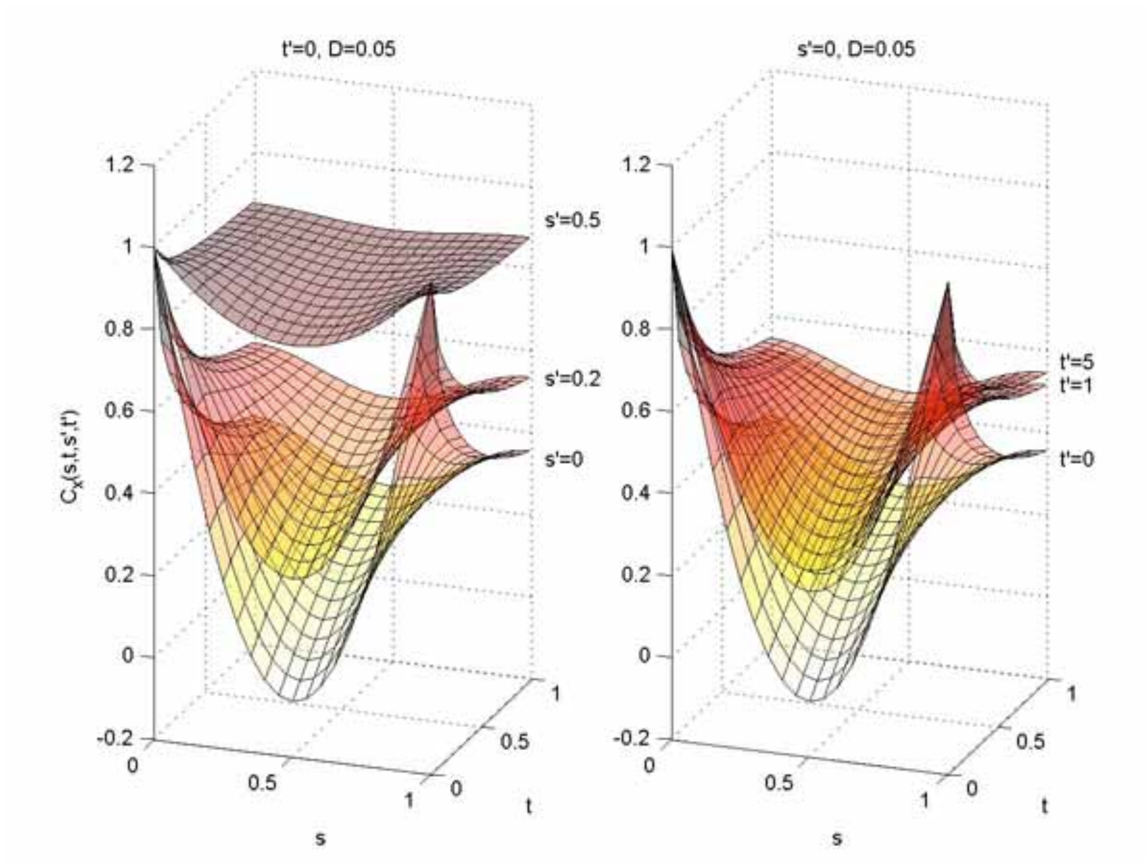
t'=0, D=0.05
s'=0, D=0.05
$C_x(s,t,s',t')$
s'=0.5
s'=0.2
s'=0
t'=5
t'=1
t'=0
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0.5
s
t

Figure 2

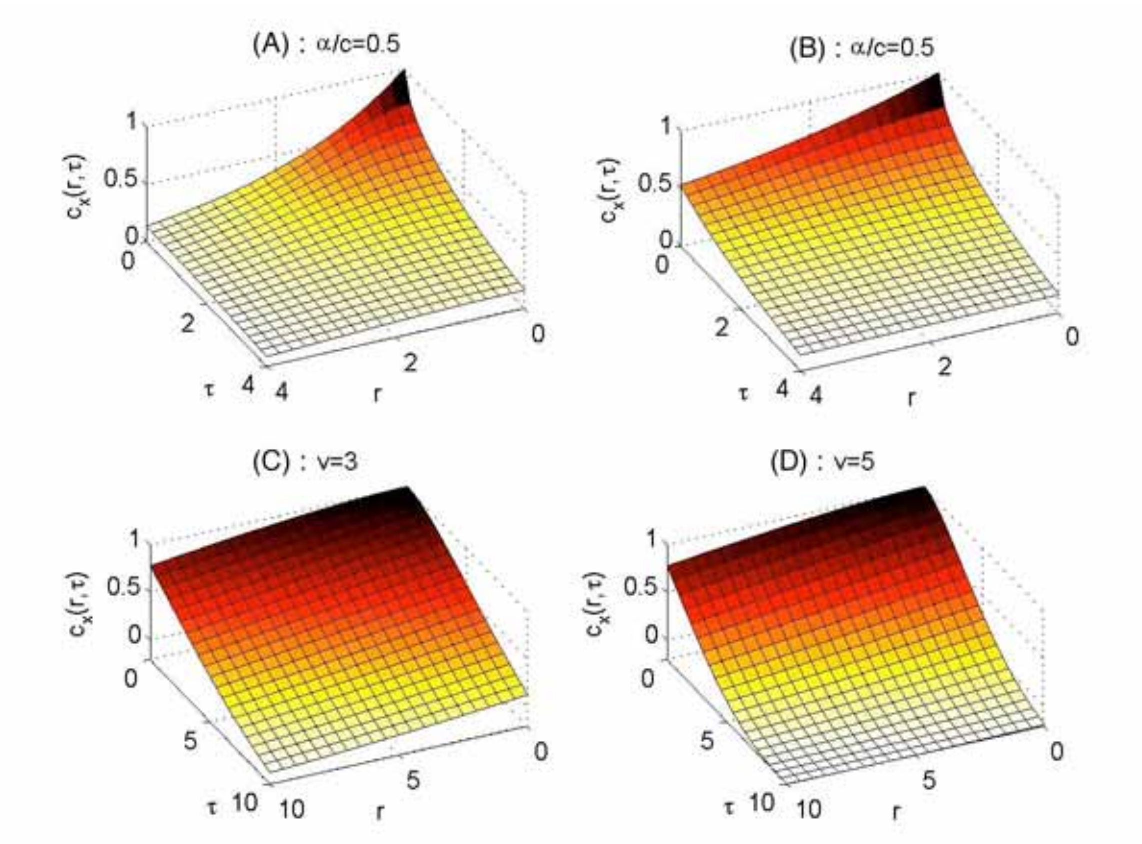

Figure 3

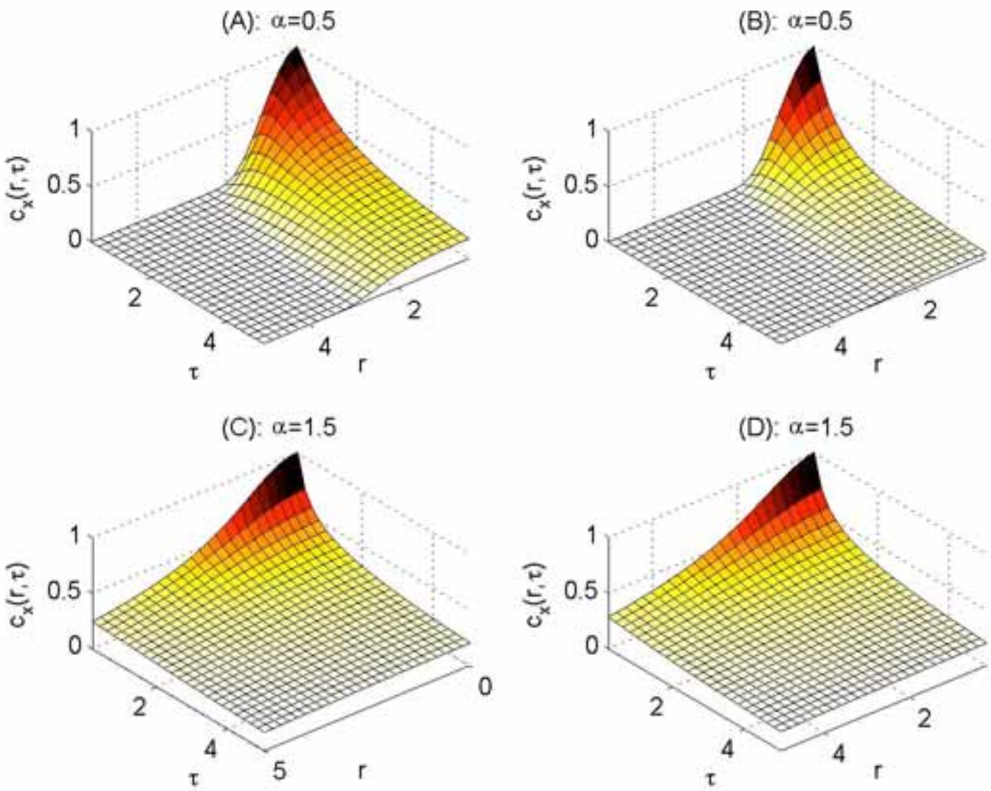

Figure 4

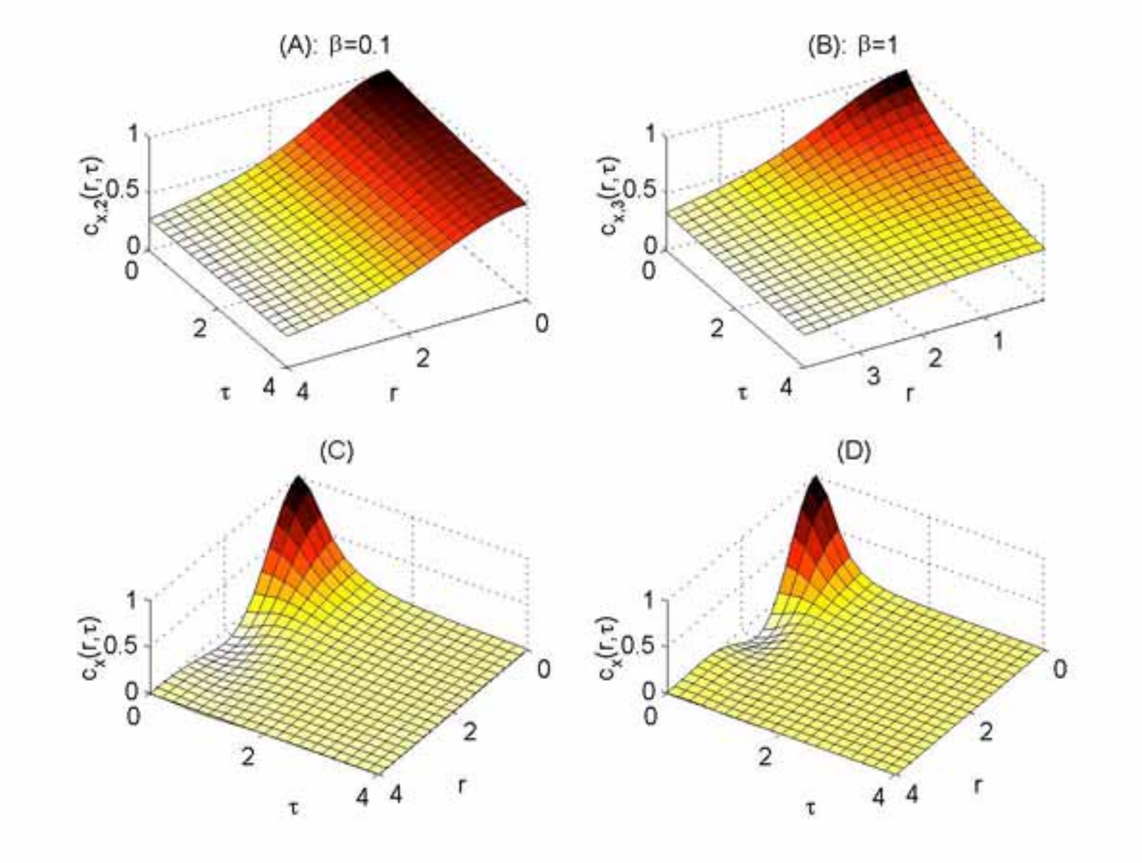

Figure 5