Probabilistic Engineering Mechanics 37 (2014) 84–92

Contents lists available at ScienceDirect

Probabilistic Engineering Mechanics

journal homepage: www.elsevier.com/locate/probengmech

Multivariate Spartan spatial random field models

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ARTICLE INFO

Article history:
Received 21 March 2014
Received in revised form
6 May 2014
Accepted 13 June 2014
Available online 21 June 2014

Keywords:
Cramer's theorem
Stationary
Multivariate spatial data
Multivariate time series
Simulation

ABSTRACT

This paper introduces a family of stationary multivariate spatial random fields with D scalar components that extend the scalar model of Gibbs random fields with local interactions (i.e., Spartan spatial random fields). We derive permissibility conditions for Spartan multivariate spatial random fields with a specific structure of local interactions. We also present explicit expressions for the respective matrix covariance functions obtained at the limit of infinite spectral cutoff in one, two and three spatial dimensions. Finally, we illustrate the proposed covariance models by means of simulated bivariate time series and two-dimensional random fields.

1. Introduction

The last thirty years have witnessed an expanding interest in spatial random field models [6,7,41] and their applications in various scientific fields that include statistics, astrophysics, hydrology, ecology, medical geography, environmental and petroleum engineering, remote sensing, and geographical information systems (GIS). This interest is motivated by the growing availability of spatial data and the need for accurate and flexible models of spatial dependence. Random field models are also applicable in mechanical engineering and computational mechanics problems [24,15,28,29,37]. There is continuing interest in the development and mathematical properties of *vector* or *multivariate random fields* (RFs for short) [36,32,30,10,13,4,31,34,35,39].

In the following, D denotes the dimension of the multivariate RF, whereas d denotes the dimension of space in which the vector field is defined. It is useful to classify multivariate RFs in two different categories. The first category includes RFs that represent distinct *physical vectors*, i.e., variables with directional dependence, such as the velocity or the force on a moving particle. The second category involves RFs that represent *composite state vectors*; the latter may comprise a number of scalar and/or vector variables, e.g., temperature, pressure, and velocity. This category also includes time series ($d=1$) of the same physical variable (e.g., wind speed), sampled at D different locations [9]; each location can be considered as a component of a D-variate vector. For physical vectors $D=d$, whereas for composite vectors it is possible that $D \gg d$; in addition, the vector components may have different units and quite different magnitudes. The matrix covariance is given by a symmetric $D \times D$ matrix which involves $D(D+1)/2$ component functions. The definition of suitable matrix covariance functions is essential for studies of correlated multi-component systems, and we expect that it will play a significant role in the analysis of scientific and engineering big data, including data from computational fluid dynamics simulations.

Let us denote by $\mathbf{v}^T = (v_1, \ldots, v_D)$ the transpose of a D-dimensional vector $\mathbf{v}$ and by $\mathbf{v} \cdot \mathbf{v}' = \sum_{i=1}^{D} v_i v_i'$ the inner product of the vectors $\mathbf{v}$ and $\mathbf{v}'$. The vector $\mathbf{s} \in \mathbb{R}^d$ denotes the position within a spatial domain of interest $\mathcal{D} \subseteq \mathbb{R}^d$. In addition, let $\mathbf{X}(\mathbf{s};\omega) = (X_1(\mathbf{s};\omega), \ldots, X_D(\mathbf{s};\omega))^T$: $\mathbb{R}^d \to \mathbb{R}^D$ be a zero-mean multivariate RF of D components $X_p(\mathbf{s};\omega), p=1,\ldots D$, defined over the probability space $(\Omega, \mathcal{F}, P)$ and indexed by the spatial variable $\mathbf{s}$ and the state variable ω. The *realizations or sample paths* of this RF will be denoted by $\mathbf{x}(\mathbf{s}) = (x_1(\mathbf{s}), \ldots, x_D(\mathbf{s}))^T$, whereas $\mathbb{E}[\cdot]$ will represent the expectation over the ensemble of the random field states. In the following we will focus on zero-mean RFs with *matrix covariance function*

$$C_{p,q}(\mathbf{s}_1, \mathbf{s}_2) := \mathbb{E}[X_p(\mathbf{s}_1;\omega) X_q(\mathbf{s}_2;\omega)], \quad p,q = 1,\ldots,d,$$

the elements of which depend only on the lag vector $\mathbf{s}_1 - \mathbf{s}_2 \in \mathbb{R}^d$. Such RFs are known as *weakly stationary, wide-sense stationary or statistically homogeneous*. We will denote the *matrix spectral density* by $\tilde{C}_{p,q}(\mathbf{k})$, where $\mathbf{k}$ is the wavevector in reciprocal (Fourier) space.

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http://dx.doi.org/10.1016/j.probengmech.2014.06.005
0266-8920/

If the multivariate RF follows the Gaussian distribution, the first two moments suffice to fully define the joint *probability density function* (pdf). Since we assume—without loss of generality—that the RF expectation is zero, one needs to specify the matrix covariance function

$$\mathbb{R}^d \ni \mathbf{r} \mapsto \mathbf{C}(\mathbf{r}) := [C_{p,q}(\mathbf{r})]_{p,q=1}^{D},$$

where $\mathbf{r}$ is the lag vector between any two points of the spatial domain, the functions $C_{p,p}(\cdot)$ are the *autocovariances* of the marginal processes $X_p(\mathbf{s};\omega)$, $p=1,\ldots,D$, and the functions $C_{p,q}(\cdot)$, where $q \neq p$ are the *cross-covariances* between the elements $X_p(\mathbf{s};\omega)$ and $X_q(\mathbf{s};\omega)$.

Scalar and matrix covariance functions must be *nonnegative definite*. A scalar function $C(\mathbf{s}_1,\mathbf{s}_2)$ is nonnegative definite if for all real vectors $\mathbf{z}=(z_1,\ldots,z_N)^T$ and all integers N the condition $\sum_{i=1}^{N}\sum_{j=1}^{N} z_i C(\mathbf{s}_i,\mathbf{s}_j)\, z_j \geq 0$ holds. In the case of scalar, weakly stationary RFs, Bochner's theorem [3] specifies the conditions for non-negative definiteness. In the case of multivariate RFs, nonnegative-definiteness requires stricter conditions as specified by Cramér's theorem [8].

Mathematically, the easiest matrix covariance construction is based on the *separability hypothesis*, i.e., $C_{p,q}(\mathbf{r}) := C(\mathbf{r}) a_{pq}$, where $C(\cdot)$ is a marginal covariance function and $A=[a_{pq}]$, $p,q=1,\ldots,D$, a nonnegative definite matrix of coefficients. The above construction is straightforward but inflexible and not supported by physical models. The popular *linear model of co-regionalization* (LMC) [17,38] is in many situations inadequate, because every vector component is represented as a linear combination of latent, independent, univariate spatial processes. In addition, the smoothness of the LMC model is dominated by the roughest of the latent components [16].

Kernel convolution methods are useful if the convolution is amenable to closed form expressions [14,27]. A class of multivariate Matérn models that extend the scalar Matérn RF is presented in [16], with generalizations in [2]. Permissibility criteria for certain matrix covariance functions are given in [33].

This paper focuses on the development of multivariate Spartan spatial RF (MSSRF) models and explicit matrix covariance functions obtained from the MSSRF covariances at the limit of infinite spectral cutoff. The MSSRFs will by construction incorporate correlations between a set of dimensionless scalar components (RFs), i.e., $X_1(\mathbf{s};\omega),\ldots,X_D(\mathbf{s};\omega)$. MSSRFs may be used to represent either distinct physical vectors or composite state vectors.

Scalar Spartan Spatial Random Fields (SSRFs) were introduced in [19]. The joint pdf of scalar SSRFs belongs to the exponential family and has certain interesting properties: (i) The respective precision (inverse covariance) matrix is based on local interactions —expressed in terms of derivatives—between the field values. This leads to sparse representations of the precision matrix. In MSSRFs, local terms will couple the vector components. (ii) In SSRFs, the permissibility condition requires that the rigidity coefficient η_1, (see (3) below) satisfies $\eta_1 > -2$. The permissibility conditions for MSSRFs are extended as described in Section 4. (iii) The inference of SSRF parameters does not require the sample-based estimation of the experimental variogram and its fit to a theoretical model, since the exponential dependence of the joint pdf and the sparsity of the precision matrix affords other options [19,22]. This property is extended to MSSRFs, which also retain the exponential density structure. (iv) SSRFs enable spatial interpolation methods which take advantage of the sparse precision matrix to reduce the computational cost of kriging [12,22]. Similar interpolation approaches for MSSRFs will be investigated in future work.

The paper is organized as follows: Section 2 reviews general properties of matrix covariance functions. Section 3 is devoted to a brief overview of scalar SSRFs. Section 4 extends the SSRF model to MSSRFs and derives explicit expressions for matrix Spartan covariance functions in $d=1,2,3$. Section 5 presents simulations of bivariate RFs with Spartan matrix covariance dependence in one and two dimensions. Finally, our conclusions and a discussion of the results are given in Section 6.

2. Preliminaries

Below we review useful mathematical properties of matrix covariance functions [38]. First, the property of *reflection symmetry* is expressed as

$$C_{p,q}(\mathbf{r}) = C_{q,p}(-\mathbf{r}), \quad p \neq q = 1,\ldots,D. \tag{1}$$

Hence, if $p \neq q$ it is not required that $C_{p,q}(\mathbf{r}) = C_{q,p}(\mathbf{r})$, which is valid only if $C_{p,q}(\mathbf{r})$ is an even function of $\mathbf{r}$.

Second, the main inequality between the diagonal and off-diagonal covariance components is

$$C_{p,p}(\mathbf{0}) C_{q,q}(\mathbf{0}) \geq |C_{p,q}(\mathbf{r})|^2.$$

Based on the Schwartz inequality it follows that $C_{p,p}(\mathbf{0}) \geq |C_{p,p}(\mathbf{r})|$. For the off-diagonal covariance functions, however, this is not necessarily true since $C_{p,q}(\mathbf{0})$ may be negative for $p \neq q$. In addition, even the inequality $|C_{p,q}(\mathbf{0})| \geq |C_{p,q}(\mathbf{r})|$ may not be true, since the maximum absolute value of the cross covariance does not have to occur at zero lag.

Third, for the matrix spectral densities, it can be shown based on Cramer's theorem [8,38] (see also Section 4) that the following inequality holds

$$|\tilde{C}_{p,q}(\mathbf{k})|^2 \leq \tilde{C}_{p,p}(\mathbf{k}) \tilde{C}_{q,q}(\mathbf{k}).$$

3. Spatial Spartan RFs for scalar-valued RFs (SSRF)

This section reviews basic facts about the construction proposed in [19]. Let $x(\mathbf{s})$ represent a state (realization) of the *scalar, zero-mean, statistically homogeneous and isotropic* $X(\mathbf{s};\omega), \mathbf{s} \in \mathcal{D} \subseteq \mathbb{R}^d$. The pdf $f_X[x(\mathbf{s})]$ is assumed to be jointly Gaussian. Isotropy implies that the *covariance function*, $C(\|\mathbf{r}\|)$, depends only on the Euclidean norm $\|\mathbf{r}\|$ of $\mathbf{r}$. The isotropy constraint can be relaxed using linear rotation and rescaling transformations; in $d=2$ this is done efficiently using the approach in [5].

3.1. SSRF Definition

The SSRF joint pdf $f_X[x(\mathbf{s})]$ is in general expressed as

$$f_X[x(\mathbf{s})] = \frac{1}{Z} e^{-H[x(\mathbf{s})]}, \tag{2}$$

where $H[x(\mathbf{s})]$ represents the *energy or cost functional* and Z is a constant that normalizes the pdf. Based on this pdf, "high-energy" states are less likely than "lower-energy" states. The role of the functional $H[\cdot]$ is to impose spatial correlations and does not necessarily represent actual energy values.

The Fluctuation-Gradient-Curvature (FGC) model is an SSRF family defined by means of the following energy functional, where η_0 is the scale parameter, η_1 is the dimensionless rigidity coefficient, and ξ is the characteristic length [19]

$$H[x(\mathbf{s})] = \frac{1}{2\eta_0 \xi^d} \int d\mathbf{s} [x^2(\mathbf{s}) + \eta_1 \xi^2 \{\nabla x(\mathbf{s})\}^2 + \xi^4 \{\nabla^2 x(\mathbf{s})\}^2]. \tag{3}$$

3.2. The concept of spectral cutoff

In order for the above energy functional to be well-defined, the fluctuations of $x(\mathbf{s})$ should be cut off above a critical wavenumber in the spectral domain. Otherwise, $C(\mathbf{r})$ becomes non-differentiable