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EOLE FOR DISCRETIZATION OF MULTIVARIATE RANDOM FIELDS

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Several engineering applications require the consideration of dependent quantities that vary randomly in space. Spatially variable dependent quantities can be modeled by means of multivariate random fields. This paper discusses methods for discretization of multivariate random fields and presents a new method based on extending the expansion optimal linear estimation (EOLE) method, originally proposed for the discretization of univariate fields. The method expresses the multivariate random field as a linear combination of uncorrelated random variables and a set of spatial vector-valued functions determined by minimizing the sum of point-wise mean-square errors of the approximation of each component of the field. The idea is based on linear estimation theory for interpolation of dependent data, i.e. the so-called co-kriging method. We discuss the properties of the method and demonstrate its applicability with a numerical example. Moreover, we show that the method can be understood as a numerical Karhunen-Loève expansion for discretization of multivariate fields.

Keywords: Multivariate random fields, discretization, correlated expansions, EOLE, co-kriging, Karhunen-Loève expansion.

1 Introduction

Many engineering applications require the consideration of physical parameters that vary randomly in space. Common examples are soil material properties in geotechnical engineering, wind and earthquake loads in structural engineering and topology of multiphase materials in bio-mechanics. This type of parameters can be modeled by means of random fields. Random fields represent infinite sets of random variables indexed by a continuous spatial parameter. If the quantity attached to each spatial point is a random variable, the field is said to be univariate. If this quantity is a random vector, the field is called multivariate. Multivariate random fields are used to describe dependent random quantities that vary randomly in space. A typical example from geotechnical engineering is the strength parameters of the soil. For example, the friction angle and cohesion of soils modeled by the Mohr-Coulomb law are typically considered to have negative point-wise correlation (Cho 2010). Recently, a number of studies have showcased the influence of the spatial variability of dependent quantities on the uncertainty and reliability of engineering systems (e.g. Cho 2010, Cho and Park 2010, Al-Bittar and Soubra 2013, Sánchez Lizarraga and Lai 2014, Babuška et al. 2014, Jiang et al. 2014).

Numerical treatment of random fields involves their approximation with a finite number of random variables. This procedure is termed random field discretization. The effi-

ciency of random field discretization methods depends on their ability to approximate accurately the random field with as few random variables as possible. Efficient random field representations involving small numbers of random variables are beneficial for most numerical methods for uncertainty quantification and reliability analysis.

Sudret and Der Kiureghian (2000) present an overview of methods for the discretization of univariate random fields. Random field discretization methods include point methods, spatial average methods and series expansion methods. In point and spatial average methods, the random field is expressed in terms of random variables that correspond to spatial points or averages of discrete parts of the spatial domain. On the other hand, series expansion methods express the random field as a superposition of products of deterministic spatial functions and random variables. That is, each random variable in the expansion has a global influence in the approximation of the random field. Through a proper choice of the spatial functions, it is often possible to describe the spatial variability accurately with much fewer terms in the expansion as compared to point or spatial average methods (Sudret and Der Kiureghian 2000). Popular series expansion methods include orthogonal series expansions (Zhang and Ellingwood 1994), the Karhunen-Loève (KL) expansion (e.g. Ghanem and Spanos 1991) and the expansion optimal linear estimation (EOLE) method (Li and Der Kiureghian 1993).

This paper addresses the discretization of multivariate random fields with series expansion methods. We first review approaches that perform multiple correlated series expansions to represent the multivariate field. Then, we discuss the application of the KL expansion to the discretization of multivariate random fields and its numerical implementation. A new method is proposed that extends the EOLE method to multivariate random fields. Moreover, it is shown that the new method can be viewed as a numerical multivariate KL expansion. The performance of the proposed method is demonstrated with a numerical example.

2 Multivariate Random Fields

Let $\mathbf{X}(\mathbf{t}) = [X_1(\mathbf{t}), X_2(\mathbf{t}), \dots, X_n(\mathbf{t})]^T$, where $\mathbf{t} \in \Omega \subset \mathbb{R}^d$, denote a n-variate d-dimensional random field. A multivariate random field is said to be second-order if the variances of its components $\mathrm{Var}\big(X_i(\mathbf{t})\big)$ exist for all $\mathbf{t} \in \Omega$ and $i = 1, \dots, n$. Second-order multivariate random fields have well-defined mean vector function $\boldsymbol{\mu}(\mathbf{t}): \Omega \longrightarrow \mathbb{R}^n$, whose element $\mu_i(\mathbf{t})$ is the mean function of $X_i(\mathbf{t})$. They also have well defined covariance matrix function $\boldsymbol{\Sigma}(\mathbf{t}, \mathbf{s}): \Omega \times \Omega \longrightarrow M_n(\mathbb{R})$, where $M_n(\mathbb{R})$ denotes the space of real $n \times n$ matrices. The (i, j) element of $\boldsymbol{\Sigma}(\mathbf{t}, \mathbf{s})$ is the covariance function

$$\Sigma_{ij}(\mathbf{t}, \mathbf{s}) = \mathrm{Cov}\big[X_i(\mathbf{t}), X_j(\mathbf{s})\big]. \qquad (1)$$

For $i = j$, $\Sigma_{ii}(\mathbf{t}, \mathbf{s})$ is the auto-covariance function of $X_i(\mathbf{t})$ and for $i \neq j$, $\Sigma_{ij}(\mathbf{t}, \mathbf{s})$ is the cross-covariance function of $X_i(\mathbf{t})$ and $X_j(\mathbf{s})$. Each covariance function can be expressed as $\Sigma_{ij}(\mathbf{t}, \mathbf{s}) = \sigma_i(\mathbf{t}) \cdot \sigma_j(\mathbf{s}) \cdot \rho_{ij}(\mathbf{t}, \mathbf{s})$, where $\sigma_i(\mathbf{t})$ is the standard deviation function of $X_i(\mathbf{t})$ and $\rho_{ij}(\mathbf{t}, \mathbf{s})$ is the correlation coefficient function of $X_i(\mathbf{t})$ and $X_j(\mathbf{s})$. The matrix-valued function $\boldsymbol{\Sigma}(\mathbf{t}, \mathbf{s})$ is symmetric, i.e., $\Sigma_{ij}(\mathbf{t}, \mathbf{s}) = \Sigma_{ji}(\mathbf{s}, \mathbf{t})$ and $\boldsymbol{\Sigma}(\mathbf{t}, \mathbf{s}) = \boldsymbol{\Sigma}(\mathbf{s}, \mathbf{t})^T$. It is also positive semi-definite, i.e.,

$$\sum_{i=1}^{m} \sum_{j=1}^{m} \mathbf{c}_i^T \boldsymbol{\Sigma}(\mathbf{t}_i, \mathbf{t}_j) \mathbf{c}_j \geq 0 \qquad (2)$$

for any $\{m, \mathbf{t}_1, \dots, \mathbf{t}_m, \mathbf{c}_1, \dots, \mathbf{c}_m\}$, $\mathbf{t}_i \in \Omega$, and $\mathbf{c}_i \in \mathbb{R}^n$. Here, we restrict our attention to second-order multivariate random fields. It is noted that the task of constructing covariance matrix functions that satisfy Eq. (2) is not straightforward (Ma 2011). Valid parametric models that extend the well-known Matérn class to cross-covariance functions are given

in (Gneiting et al. 2010, Apanasovich et al. 2012).

3 Error Measures for Random Field Discretization

The approximation $\widehat{\mathbf{X}}(\mathbf{t})$ of a continuous random field $\mathbf{X}(\mathbf{t})$ by a finite set of random variables $\{\xi_i, i = 1, \dots, m\}$ is termed random field discretization. The approximation error $\boldsymbol{\epsilon}(\mathbf{t})$ is defined as the difference between the original field and its approximation, i.e., $\boldsymbol{\epsilon}(\mathbf{t}) = \mathbf{X}(\mathbf{t}) - \widehat{\mathbf{X}}(\mathbf{t})$. Define a matrix-valued function $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t}): \Omega \longrightarrow M_n(\mathbb{R})$ having the elements $\Sigma_{\epsilon,ij}(\mathbf{t}) = \mathrm{Cov}\big[\epsilon_i(\mathbf{t}), \epsilon_j(\mathbf{t})\big]$. That is, $\Sigma_{\epsilon,ij}(\mathbf{t})$ is the point-wise covariance of $\epsilon_i(\mathbf{t})$ and $\epsilon_j(\mathbf{t})$ so that the ith diagonal element of $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ represents the variance of the error of the representation $\hat{X}_i(\mathbf{t})$ of $X_i(\mathbf{t})$. It is reasonable to assume that the mean of the vector field $\mathbf{X}(\mathbf{t})$ can be represented exactly. In this case, the elements of $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ also equal $\Sigma_{\epsilon,ij}(\mathbf{t}) = \mathrm{E}\big[\epsilon_i(\mathbf{t})\epsilon_j(\mathbf{t})\big]$. That is, the ith diagonal element of $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ is equal to the point-wise mean square of the approximation error of $\hat{X}_i(\mathbf{t})$.

For assessing the accuracy of the discretization method, we defined the following point-wise relative error for each pair of components (i, j) of the vector field:

$$\delta_{ij}(\mathbf{t}) = \frac{\Sigma_{\epsilon,ij}(\mathbf{t})}{\mathrm{Cov}\big[X_i(\mathbf{t}), X_j(\mathbf{t})\big]} = \frac{\mathrm{Cov}\big[X_i(\mathbf{t}) - \hat{X}_i(\mathbf{t}), X_j(\mathbf{t}) - \hat{X}_j(\mathbf{t})\big]}{\mathrm{Cov}\big[X_i(\mathbf{t}), X_j(\mathbf{t})\big]}. \quad (3)$$

For $i = j$, $\delta_{ii}(\mathbf{t})$ reflects the mean-square relative accuracy of the approximation of each component field $\hat{X}_i(\mathbf{t})$ at each point $\mathbf{t}$ and for $i \neq j$, $\delta_{ij}(\mathbf{t})$ reflects the linear dependence between the errors in approximation $\hat{X}_i(\mathbf{t})$ and $\hat{X}_j(\mathbf{t})$ at point $\mathbf{t}$. We also define the corresponding global errors as the spatial average of the point-wise errors, given by

$$\bar{\delta}_{ij} = \frac{1}{|\Omega|}\int_{\Omega} \delta_{ij}(\mathbf{t}) d\mathbf{t}. \quad (4)$$

4 Multiple Correlated Series Expansions

Consider a particular class of multivariate random fields whose components have identical auto-correlation coefficient functions $\rho(\mathbf{t}, \mathbf{s})$ and each cross-correlation coefficient function $\rho_{ij}(\mathbf{t}, \mathbf{s})$ is given by the following proportional model:

$$\rho_{ij}(\mathbf{t}, \mathbf{s}) = \rho_{ij}^c \cdot \rho(\mathbf{t}, \mathbf{s}) \quad (5)$$

where ρ_{ij}^c is the point-wise cross-correlation of $X_i(\mathbf{t})$ and $X_j(\mathbf{t})$. That is, the cross-correlation between each pair of random fields at the same location $\mathbf{t}$ is constant and equals ρ_{ij}^c. Vořechovský (2008) proposed to discretize multivariate fields belonging to this class through performing the series expansion of each component $X_i(\mathbf{t})$ and imposing a correlation between random variables derived from different expansions. For the discretization of each random field $X_i(\mathbf{t})$, Vořechovský (2008) proposed to apply either the univariate KL expansion or the EOLE method. The truncated KL expansion $\hat{X}_i(\mathbf{t})$ of component field $X_i(\mathbf{t})$ reads:

$$\hat{X}_i(\mathbf{t}) = \mu_i(\mathbf{t}) + \sum_{k=1}^{m} \xi_k^i \sqrt{\lambda_k^i}\varphi_k^i(\mathbf{t}) \quad (6)$$

where $\{\lambda_k^i, \varphi_k^i(\mathbf{t})\}$ are the eigenpairs of the auto-covariance function $\Sigma_{ii}(\mathbf{t}, \mathbf{s})$. The corresponding EOLE representation $\hat{X}_i(\mathbf{t})$ of the field $X_i(\mathbf{t})$ reads:

$$\hat{X}_i(\mathbf{t}) = \mu_i(\mathbf{t}) + \sum_{k=1}^{m} \frac{\xi_k^i}{\sqrt{\lambda_k^i}} \boldsymbol{\Sigma}_q^i(\mathbf{t})^T \boldsymbol{\Phi}_k^i \quad (7)$$

Here, $\{\lambda_k^i, \boldsymbol{\Phi}_k^i\}$ are the eigenpairs of the covariance matrix of the random variables $X_i(\mathbf{t}_j)$ corresponding to a set of points $\{\mathbf{t}_j, j = 1, \dots, q\}$ and $\boldsymbol{\Sigma}_q^i(\mathbf{t})$ is a $q \times 1$ vector function with j element $\Sigma_{ii}(\mathbf{t}, \mathbf{t}_j)$. In both series expansions, the variables $\{\xi_k^i, k = 1, \dots, m\}$ are zero mean orthonormal random variables. Using either of the two expansions to represent each component field, we can model the cross-correlation function of Eq. (5) through introducing a correlation between each pair $\{\xi_k^i, \xi_l^j\}$ for $k = l$. That is,

$$\mathrm{E}[\xi_k^i \xi_l^j] = \begin{cases} \delta_{kl} & , i = j \\ \rho_{ij}^c \delta_{kl} & , i \neq j \end{cases} \tag{8}$$

where δ_{ij} is the Kronecker delta. The approach of (Vořechovský 2008) has the limitation that it can only represent multivariate random fields with identical auto-correlation functions and cross-correlation function of the form of Eq. (5). Cho et al. (2013) generalized the idea of using multiple correlated series expansion to multivariate random fields with arbitrary covariance matrix function. Their method performs the KL expansion of each component field and evaluates the correlation between variables derived from different expansions through projecting the cross-covariance functions to the eigenfunction set of each component field. That is,

$$\mathrm{E}[\xi_k^i \xi_l^j] = \frac{1}{\sqrt{\lambda_k^i \lambda_l^j}} \int_\Omega \int_\Omega \Sigma_{ij}(\mathbf{t}, \mathbf{s}) \varphi_k^i(\mathbf{t}) \varphi_l^j(\mathbf{s}) d\mathbf{t} d\mathbf{s} \tag{9}$$

The cross-covariance function $\hat{\Sigma}_{ij}(\mathbf{t}, \mathbf{s})$ of the approximated vector field then reads:

$$\hat{\Sigma}_{ij}(\mathbf{t}, \mathbf{s}) = \sum_{k=1}^{m} \sum_{l=1}^{m} \mathrm{E}[\xi_k^i \xi_l^j] \sqrt{\lambda_k^i \lambda_l^j} \varphi_k^i(\mathbf{t}) \varphi_l^j(\mathbf{s}) \tag{10}$$

It is noted here that the same concept can be applied in the case where each component field is approximated by the EOLE representation of Eq. (7). In this case, the correlation between each pair of random variables $\{\xi_k^i, \xi_l^j\}$ for $i \neq j$ can be evaluated as

$$\mathrm{E}[\xi_k^i \xi_l^j] = \frac{1}{\sqrt{\lambda_k^i \lambda_l^j}} \left(\boldsymbol{\Phi}_k^i\right)^T \boldsymbol{\Sigma}^{ij} \boldsymbol{\Phi}_l^j \tag{11}$$

where $\boldsymbol{\Sigma}^{ij}$ is a $q \times q$ cross-covariance matrix with (k, l) element $\Sigma_{ij}(\mathbf{t}_k, \mathbf{t}_l)$. The corresponding approximation of each cross-covariance function reads:

$$\hat{\Sigma}_{ij}(\mathbf{t}, \mathbf{s}) = \sum_{k=1}^{m} \sum_{l=1}^{m} \frac{\mathrm{E}[\xi_k^i \xi_l^j]}{\sqrt{\lambda_k^i \lambda_l^j}} \boldsymbol{\Sigma}_q^i(\mathbf{t})^T \boldsymbol{\Phi}_k^i \boldsymbol{\Sigma}_q^j(\mathbf{s})^T \boldsymbol{\Phi}_l^j \tag{12}$$

To represent the vector field accurately, one needs to choose the number of random variables such that the errors defined in Eq. (4) are small. When using multiple correlated series expansion, the global mean-square error $\bar{\delta}_{ii}$ of each component field $X_i(\mathbf{t})$ for a given number of terms in the expansion depends on the autocorrelation function of $X_i(\mathbf{t})$. If the component field is highly fluctuating, a large number of terms are required to achieve a small mean square error. On the other hand, slowly varying fields can be represented accurately with just a few terms. However, the cross-covariance functions introduce dependence between each pair of component random fields and hence decrease their relative variability. It is possible to account for the cross-covariance in choosing the spatial functions in the series expansion, hence decreasing the number of random variables needed to represent accurately the multivariate field. Next, we look at series expansion methods that account for this dependence.

5 Karhunen-Loève Expansion of Multivariate Random Fields

Consider the Hilbert space $L^2(\Omega, \mathbb{R}^n)$ of square integrable vector-valued functions $\mathbf{f}(\mathbf{t}): \Omega \longrightarrow \mathbb{R}^n$, i.e. $\mathbf{f}(\mathbf{t})$ satisfying

$$\|\mathbf{f}\| = \sqrt{\langle \mathbf{f}, \mathbf{f} \rangle} < \infty \tag{13}$$

where $\langle \cdot, \cdot \rangle$ is the inner product on $L^2(\Omega, \mathbb{R}^n)$ defined by:

$$\langle \mathbf{f}, \mathbf{g} \rangle = \int_{\Omega} \mathbf{f}(\mathbf{t})^T \mathbf{g}(\mathbf{t}) d\mathbf{t} \tag{14}$$

Assuming that $\mathbf{\Sigma}(\mathbf{t}, \mathbf{s})$ is continuous and that its elements are square integrable functions, then according to Mercer's theorem for vector valued functions (Carmeli et. al. 2006), the kernel $\mathbf{\Sigma}(\mathbf{t}, \mathbf{s})$ adheres the spectral decomposition

$$\mathbf{\Sigma}(\mathbf{t}, \mathbf{s}) = \sum_{i=1}^{\infty} \lambda_i \boldsymbol{\varphi}_i(\mathbf{t}) \boldsymbol{\varphi}_i(\mathbf{s})^T \tag{15}$$

where $\{\boldsymbol{\varphi}_i, i \in \mathbb{N}\}$ is an orthonormal basis of $L^2(\Omega, \mathbb{R}^n)$, i.e.

$$\langle \boldsymbol{\varphi}_i, \boldsymbol{\varphi}_j \rangle = \delta_{ij} \tag{16}$$

and $\{\lambda_i, i \in \mathbb{N}\}$ are non-negative real numbers arranged in a decreasing order, i.e. $\lambda_1 \geq \lambda_2 \geq \cdots$. The pairs $\{\lambda_i, \boldsymbol{\varphi}_i\}$ are the eigenvalues and eigenfunctions of $\mathbf{\Sigma}(\mathbf{t}, \mathbf{s})$ and satisfy the following system of integral equations:

$$\int_{\Omega} \mathbf{\Sigma}(\mathbf{t}, \mathbf{s}) \boldsymbol{\varphi}_i(\mathbf{s}) d\mathbf{s} = \lambda_i \boldsymbol{\varphi}_i(\mathbf{t}) \tag{17}$$

for all $i \in \mathbb{N}$, wherein the integration is performed element-wise. The KL expansion of the vector field $\mathbf{X}(\mathbf{t})$ truncated after the m largest eigenvalues reads (e.g. Busch et al. 2011, Perrin et al. 2013):

$$\widehat{\mathbf{X}}(\mathbf{t}) = \boldsymbol{\mu}(\mathbf{t}) + \sum_{i=1}^{m} \xi_i \sqrt{\lambda_i} \boldsymbol{\varphi}_i(\mathbf{t}) \tag{18}$$

where $\{\xi_i\}$ are zero mean orthonormal random variables, given in the following closed form

$$\xi_i = \frac{1}{\sqrt{\lambda_i}} \int_{\Omega} \boldsymbol{\varphi}_i(\mathbf{t})^T \big(\mathbf{X}(\mathbf{t}) - \boldsymbol{\mu}(\mathbf{t})\big) d\mathbf{t} \tag{19}$$

From Eq. (19) it is clear that if the vector field is Gaussian, then the random variables $\{\xi_i\}$ are also Gaussian, because they are defined as a linear mapping of a Gaussian field. In this case, the variables $\{\xi_i\}$ are independent standard normal random variables.

The mean function of $\widehat{\mathbf{X}}(\mathbf{t})$ equals the mean of $\mathbf{X}(\mathbf{t})$ by definition. The matrix-valued covariance function of $\widehat{\mathbf{X}}(\mathbf{t})$ reads:

$$\widehat{\mathbf{\Sigma}}(\mathbf{t}, \mathbf{s}) = \sum_{i=1}^{m} \lambda_i \boldsymbol{\varphi}_i(\mathbf{t}) \boldsymbol{\varphi}_i(\mathbf{s})^T \tag{20}$$

The covariance matrix function $\mathbf{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ of the truncation error of the representation of Eq. (18) can be expressed as:

$$\mathbf{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t}) = \mathbf{\Sigma}(\mathbf{t}, \mathbf{t}) - \sum_{i=1}^{m} \lambda_i \boldsymbol{\varphi}_i(\mathbf{t}) \boldsymbol{\varphi}_i(\mathbf{t})^T \tag{21}$$

The second term in the above is identical to $\widehat{\mathbf{\Sigma}}(\mathbf{t}, \mathbf{s})$. Since the diagonal elements of $\mathbf{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ are always positive, it follows that each element $\hat{X}_i(\mathbf{t})$ of the approximate multivariate field $\widehat{\mathbf{X}}(\mathbf{t})$ always underestimates the pointwise variance of the corresponding element of the original field. This property of the KL expansion was discussed in (Sudret and Der Kiureghian 2000) for the case of univariate random fields.

It can be shown that the expansion of Eq. (18) is optimal in the sense that the integral of

trace of the matrix function $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$, i.e. the integral of the sum of the mean square errors of the approximated random fields is minimized for the particular choice of the eigenfunctions of $\boldsymbol{\Sigma}(\mathbf{t},\mathbf{s})$ relative to any other orthonormal basis in $L^2(\Omega,\mathbb{R}^n)$.

5.1 *Numerical Solution of the Eigenvalue Problem*

It is highly unlikely that the matrix-valued integral eigenvalue problem in Eq. (17) will have an analytical solution for an arbitrarily selected covariance matrix function of the multivariate random field. In this section, we discuss a method for numerical solution of this problem. In a subsequent section we show that one particular case of this solution is equivalent to the EOLE method, which is described in the next section.

Equation (17) represents a system of n Fredholm integral equations and can be solved by a variety of numerical methods (see Atkinson 1997, Betz et al. 2014). Here, we describe the Nyström method (see, e.g. Atkinson 1997). According to this method, the integrals in Eq. (17) are approximated by a quadrature scheme so that

$$\sum_{j=1}^{q} w_j \boldsymbol{\Sigma}(\mathbf{t},\mathbf{t}_j)\boldsymbol{\varphi}_i(\mathbf{t}_j) = \lambda_i \boldsymbol{\varphi}_i(\mathbf{t}), \qquad (22)$$

where $\{\mathbf{t}_j, w_j\}$, $j = 1,\dots,q$, are a set of nodes and corresponding weights and convergence to the true integrals in Eq. (17) is achieved as $q \to \infty$. Note that we are using the same set $\{\mathbf{t}_j, w_j\}$ for approximating all integrals in Eq. (17). Requiring that Eq. (22) is satisfied at the quadrature nodes $\mathbf{t}_k$, $k = 1,\dots,q$, yields:

$$\sum_{j=1}^{q} w_j \boldsymbol{\Sigma}(\mathbf{t}_k,\mathbf{t}_j)\boldsymbol{\varphi}_i(\mathbf{t}_j) = \lambda_i \boldsymbol{\varphi}_i(\mathbf{t}_k), \quad k = 1,\dots,q \qquad (23)$$

The above is a matrix eigensystem of order qn and can be expressed in matrix form as

$$\boldsymbol{\Sigma}\mathbf{W}\boldsymbol{\Phi}_i = \lambda_i \boldsymbol{\Phi}_i \qquad (24)$$

where $\boldsymbol{\Sigma}$ and $\mathbf{W}$ are $qn \times qn$ matrices defined as

$$\boldsymbol{\Sigma} := \begin{bmatrix} \boldsymbol{\Sigma}(\mathbf{t}_1,\mathbf{t}_1) & \cdots & \boldsymbol{\Sigma}(\mathbf{t}_1,\mathbf{t}_q) \\ \vdots & \ddots & \vdots \\ \boldsymbol{\Sigma}(\mathbf{t}_q,\mathbf{t}_1) & \cdots & \boldsymbol{\Sigma}(\mathbf{t}_q,\mathbf{t}_q) \end{bmatrix} \qquad (25)$$

and

$$\mathbf{W} := \begin{bmatrix} w_1\mathbf{I} & \cdots & \mathbf{0} \\ \vdots & \ddots & \vdots \\ \mathbf{0} & \cdots & w_q\mathbf{I} \end{bmatrix}, \qquad (26)$$

where $\mathbf{I}$ is the $n \times n$ identity matrix, and $\boldsymbol{\Phi}_i$ is the $qn \times 1$ vector

$$\boldsymbol{\Phi}_i := \begin{bmatrix} \boldsymbol{\varphi}_i(\mathbf{t}_1) \\ \vdots \\ \boldsymbol{\varphi}_i(\mathbf{t}_q) \end{bmatrix}. \qquad (27)$$

The product $\boldsymbol{\Sigma}\mathbf{W}$ leads to an asymmetric matrix eigenvalue problem; however, it can be transformed to a symmetric problem by left-multiplying Eq. (24) with $\mathbf{W}^{1/2}$ (Press et al. 1992), as follows:

$$\mathbf{W}^{1/2}\boldsymbol{\Sigma}\mathbf{W}^{1/2}\boldsymbol{\Phi}_i^* = \lambda_i \boldsymbol{\Phi}_i^* \qquad (28)$$

where $\boldsymbol{\Phi}_i^* = \mathbf{W}^{1/2}\boldsymbol{\Phi}_i$. The resulting symmetric matrix eigenvalue problem is solved for the qn positive eigenvalues λ_i and corresponding eigenvectors $\boldsymbol{\Phi}_i^*$. The eigenfunctions $\boldsymbol{\varphi}_i(\mathbf{t})$ are then approximated by using the Nyström interpolation formula, derived by solving Eq. (22) for $\boldsymbol{\varphi}_i(\mathbf{t})$, which gives

$$\boldsymbol{\varphi}_i(\mathbf{t}) = \frac{1}{\lambda_i}\boldsymbol{\Sigma}_q(\mathbf{t})^T\mathbf{W}^{1/2}\boldsymbol{\Phi}_i^*, \qquad (29)$$

in which $\boldsymbol{\Sigma}_q(\mathbf{t})$ is the following $qn \times n$ matrix-valued function:

$$\boldsymbol{\Sigma}_q(\mathbf{t}) := \begin{bmatrix} \boldsymbol{\Sigma}(\mathbf{t},\mathbf{t}_1) \\ \vdots \\ \boldsymbol{\Sigma}(\mathbf{t},\mathbf{t}_q) \end{bmatrix}. \qquad (30)$$

6 EOLE of Multivariate Random Fields

We now consider an entirely different approach for discretizing second-order multivariate random fields. In the subsequent section, we show that this formulation is equivalent to the numerical solution of the multivariate KL expansion using Nyström's method with uniform weights.

We start by constructing an approximation $\widehat{\mathbf{X}}(\mathbf{t})$ of the random field $\mathbf{X}(\mathbf{t})$, defined as a linear function of the random vectors $\mathbf{X}(\mathbf{t}_i)$ corresponding to a set of nodes $\mathbf{t}_i$, $i = 1, \dots, q$, i.e.,

$$\widehat{\mathbf{X}}(\mathbf{t}) = \mathbf{a}(\mathbf{t}) + \mathbf{B}(\mathbf{t})^T \mathbf{X}_q \tag{31}$$

where $\mathbf{a}(\mathbf{t}): \Omega \longrightarrow \mathbb{R}^n$, $\mathbf{B}(\mathbf{t})$ is the $qn \times n$ matrix-valued function:

$$\mathbf{B}(\mathbf{t}) := \begin{bmatrix} \mathbf{b}_1(\mathbf{t}) \\ \vdots \\ \mathbf{b}_q(\mathbf{t}) \end{bmatrix}, \tag{32}$$

where $\mathbf{b}_i(\mathbf{t}): \Omega \longrightarrow M_n(\mathbb{R})$, and $\mathbf{X}_q$ is the $qn \times 1$ vector of random variables

$$\mathbf{X}_q := \begin{bmatrix} \mathbf{X}(\mathbf{t}_1) \\ \vdots \\ \mathbf{X}(\mathbf{t}_q) \end{bmatrix}. \tag{33}$$

The functions $\mathbf{a}(\mathbf{t})$ and $\mathbf{B}(\mathbf{t})$ are determined by application of linear estimation theory for interpolation of dependent data, i.e. the so-called co-kriging method (e.g. see Stein 1999). Define $\boldsymbol{\epsilon}(\mathbf{t})$ as the point-wise error of the approximation in Eq. (31), i.e. $\boldsymbol{\epsilon}(\mathbf{t}) = \mathbf{X}(\mathbf{t}) - \widehat{\mathbf{X}}(\mathbf{t})$. Let $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ be the $n \times n$ matrix-valued covariance function of $\boldsymbol{\epsilon}(\mathbf{t})$ and recall that the ith diagonal element of $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ is the variance of the error in the approximate representation of $X_i(\mathbf{t})$. We seek the functions $\mathbf{a}(\mathbf{t})$, $\mathbf{B}(\mathbf{t})$ that minimize the trace of $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ subject to $\widehat{\mathbf{X}}(\mathbf{t})$ being an unbiased estimator of $\mathbf{X}(\mathbf{t})$, i.e.,

$$\text{minimize} \quad \text{tr}\big(\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})\big) \tag{34}$$

$$\text{subject to} \quad \text{E}[\boldsymbol{\epsilon}(\mathbf{t})] = \mathbf{0} \tag{35}$$

From Eq. (35), we have

$$\mathbf{a}(\mathbf{t}) = \boldsymbol{\mu}(\mathbf{t}) - \mathbf{B}(\mathbf{t})^T \mathbf{M} \tag{36}$$

where $\mathbf{M}$ is the $qn \times 1$ mean vector of $\mathbf{X}_q$,

$$\mathbf{M} := \begin{bmatrix} \boldsymbol{\mu}(\mathbf{t}_1) \\ \vdots \\ \boldsymbol{\mu}(\mathbf{t}_q) \end{bmatrix}. \tag{37}$$

The error covariance $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ can then be written as

$$\begin{aligned} \boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t}) &= \boldsymbol{\Sigma}(\mathbf{t}, \mathbf{t}) + \mathbf{B}(\mathbf{t})^T \boldsymbol{\Sigma} \mathbf{B}(\mathbf{t}) \\ &\quad - 2 \cdot \mathbf{B}(\mathbf{t})^T \boldsymbol{\Sigma}_q(\mathbf{t}), \end{aligned} \tag{38}$$

where $\boldsymbol{\Sigma}$ and $\boldsymbol{\Sigma}_q(\mathbf{t})$ are defined in Eq. (25) and Eq. (30), respectively. Taking the partial derivative of the trace of $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ in terms of each element of $\mathbf{B}(\mathbf{t})$ and setting it equal to zero, yields:

$$\begin{aligned} \frac{\partial \text{tr}(\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t}))}{\partial \mathbf{B}(\mathbf{t})} &= 2 \cdot \boldsymbol{\Sigma} \mathbf{B}(\mathbf{t}) - 2 \cdot \boldsymbol{\Sigma}_q(\mathbf{t}) \\ &= \mathbf{0} \end{aligned} \tag{39}$$

which yields $\mathbf{B}(\mathbf{t}) = \boldsymbol{\Sigma}^{-1} \boldsymbol{\Sigma}_q(\mathbf{t})$. Substituting this result together with Eq. (36) in Eq. (31), we obtain the following optimal linear estimation (OLE) representation of $\mathbf{X}(\mathbf{t})$:

$$\widehat{\mathbf{X}}(\mathbf{t}) = \boldsymbol{\mu}(\mathbf{t}) + \boldsymbol{\Sigma}_q(\mathbf{t})^T \boldsymbol{\Sigma}^{-1} \big(\mathbf{X}_q - \mathbf{M}\big) \tag{40}$$

Equation (40) is a generalization of the OLE method for discretization of univariate random fields presented by Li and Der Kiureghian (1993). In the same reference, the authors proposed the expansion optimal linear estimation (EOLE) method, which is based on the spectral decomposition of the covariance matrix $\boldsymbol{\Sigma}$ of the nodal random variables. Using the same concept, here we develop the EOLE of multivariate fields.

The nodal vector of random variables, $\mathbf{X}_q$, can be expressed as follows (e.g. see Yamazaki and Shinozuka 1990):

$$\mathbf{X}_q = \mathbf{M} + \sum_{i=1}^{qn} \xi_i \sqrt{\lambda_i} \boldsymbol{\Phi}_i \tag{41}$$

where $\{\lambda_i, \boldsymbol{\Phi}_i\}, i = 1, \dots, q$, are the eigenvalues and corresponding eigenvectors of the covariance matrix $\boldsymbol{\Sigma}$ satisfying

$$\boldsymbol{\Sigma}\boldsymbol{\Phi}_i = \lambda_i \boldsymbol{\Phi}_i, \quad i = 1, \dots, nq \tag{42}$$

and $\{\xi_i\}$ are zero mean orthonormal random variables defined as

$$\xi_i = \frac{1}{\sqrt{\lambda_i}} \boldsymbol{\Phi}_i^T (\mathbf{X}_q - \mathbf{M}). \tag{43}$$

If the vector field is Gaussian, then the random vector $\mathbf{X}_q$ is also Gaussian and so are the random variables $\{\xi_i\}$, because they are defined as a linear mapping of $\mathbf{X}_q$. In this case, the variables $\{\xi_i\}$ are independent standard normal random variables. A truncation of the sum in Eq. (41) after m terms leads to an approximation of the random vector $\mathbf{X}_q$, which corresponds to the optimal low rank approximation of the covariance matrix $\boldsymbol{\Sigma}$ in terms of its Frobenius norm, according to the Eckart-Young theorem (see, e.g. Stewart 1993). Substituting Eq. (41), truncated after m terms into Eq. (31) and solving the OLE optimization problem, we get:

$$\widehat{\mathbf{X}}(\mathbf{t}) = \boldsymbol{\mu}(\mathbf{t}) + \sum_{i=1}^{m} \frac{\xi_i}{\sqrt{\lambda_i}} \boldsymbol{\Sigma}_q(\mathbf{t})^T \boldsymbol{\Phi}_i \tag{44}$$

The mean function of $\widehat{\mathbf{X}}(\mathbf{t})$ equals the mean of $\mathbf{X}(\mathbf{t})$. The matrix-valued covariance function of $\widehat{\mathbf{X}}(\mathbf{t})$ reads:

$$\widehat{\boldsymbol{\Sigma}}(\mathbf{t}, \mathbf{s}) = \sum_{i=1}^{m} \frac{1}{\lambda_i} \boldsymbol{\Sigma}_q(\mathbf{t})^T \boldsymbol{\Phi}_i \boldsymbol{\Phi}_i^T \boldsymbol{\Sigma}_q(\mathbf{s}). \tag{45}$$

The covariance matrix function $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$ of the error of the representation of Eq. (44) reads

$$\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t}) = \boldsymbol{\Sigma}(\mathbf{t}, \mathbf{t}) - \sum_{i=1}^{m} \frac{1}{\lambda_i} \boldsymbol{\Sigma}_q(\mathbf{t})^T \boldsymbol{\Phi}_i \boldsymbol{\Phi}_i^T \boldsymbol{\Sigma}_q(\mathbf{t}). \tag{46}$$

The second term in the above is identical to $\widehat{\boldsymbol{\Sigma}}(\mathbf{t}, \mathbf{t})$. Therefore, similar to the KL representation, the EOLE representation for multivariate random fields underestimates the variance of each component random field, $X_i(\mathbf{t})$. Li and Der Kiureghian (1993) made this observation for the EOLE representation of univariate random fields.

6.1 *EOLE as a Numerical Solution of the KL Expansion*

In Section 5.1, we described the Nyström method for the numerical solution of the KL eigenvalue problem. Here, we show that the EOLE for multivariate random fields can be seen as a numerical KL expansion for the case where the system of Fredholm eigenvalue equations is solved by the Nyström method. The same is shown by Betz et al. (2014) for the case of univariate random fields.

In the Nyström method, the integral eigenvalue problem of Eq. (17) is approximated by a finite sum, as shown in Eq. (22). Assume that the quadrature nodes are selected such that their weights are equal. This can be done, for example, by application of the rectangle quadrature using the nodes of an equispaced structured grid. In that case, the approximated eigenvalue problem takes the form

$$\frac{|\Omega|}{q} \sum_{j=1}^{q} \boldsymbol{\Sigma}(\mathbf{t}, \mathbf{t}_j) \boldsymbol{\varphi}_i(\mathbf{t}_j) = \lambda_i \boldsymbol{\varphi}_i(\mathbf{t}). \tag{47}$$

Requiring that Eq. (47) be satisfied at the nodes $\mathbf{t}_i$, $i = 1, \dots, q$, leads to the following eigenvalue problem:

$$\frac{|\Omega|}{q}\mathbf{\Sigma}\mathbf{\Phi}_i^* = \lambda_i \mathbf{\Phi}_i^* \tag{48}$$

where $\mathbf{\Sigma}$ is defined in Eq. (25). Solving Eq. (48) and substituting in the Nyström interpolation formula of Eq. (29), we have:

$$\boldsymbol{\varphi}_i(\mathbf{t}) = \frac{1}{\lambda_i}\sqrt{\frac{|\Omega|}{q}}\mathbf{\Sigma}_q(\mathbf{t})^T\mathbf{\Phi}_i^* \tag{49}$$

Substituting this result in Eq. (18), we get the following expression for the approximate KL representation of $\mathbf{X}(\mathbf{t})$:

$$\hat{\mathbf{X}}(\mathbf{t}) = \boldsymbol{\mu}(\mathbf{t}) + \sum_{i=1}^{m}\frac{\xi_i}{\sqrt{\lambda_i^*}}\mathbf{\Sigma}_q(\mathbf{t})^T\mathbf{\Phi}_i^* \tag{50}$$

where $\lambda_i^* = \frac{\lambda_i q}{|\Omega|}$. Note that $\{\lambda_i^*, \mathbf{\Phi}_i^*\}$ are the eigenvalues and corresponding eigenvectors of the matrix $\mathbf{\Sigma}$ and thus Eq. (50) is identical to Eq. (44). Hence, the EOLE expansion is a numerical approximation of the KL expansion and will converge to the analytical KL expansion as $q \to \infty$.

7 Numerical Example

This example consists of a bivariate one-dimensional homogeneous standard Gaussian random field defined in $\Omega = [0,10]$. We adopt the exponential model to describe the auto-correlation structures of each component field, i.e.

$$\Sigma_{ii}(\tau) = \exp(-a_{ii}|\tau|) \tag{51}$$

where τ is the difference in location between two points $a_{ii} = \frac{1}{l_{ii}}$, and l_{ii} is the correlation length of component field $X_i(\mathbf{t})$. The correlation lengths are chosen as $l_{11} = 10$ and $l_{22} = 5$. The cross-correlation structure is also given by the exponential model, so that

$$\Sigma_{12}(\tau) = \rho_{12}^c \exp(-a_{12}|\tau|) \tag{52}$$

where ρ_{12}^c is the point-wise cross-correlation of the two fields, chosen as $\rho_{12}^c = 0.7$. The parameter a_{12} is chosen as $a_{12} = \frac{a_{11}+a_{12}}{2}$, which leads to a valid covariance matrix function – the conditions under which the exponential model is valid can be found in (Apanasovich et al. 2012).

The multivariate EOLE and KL methods are applied to discretize the random field and we compare the accuracies of the two methods. For the EOLE, we use 20 equispaced nodes for the point representation of the random field. For the KL, we solve the integral equation system of Eq. (17) with the Nyström method with 200 equispaced quadrature points, which is equivalent to the EOLE method with 200 points (see Section 6.1). Figures 1-3 show the point-wise relative errors of Eq. (3) for the two discretization methods. It is shown that the point-wise errors of the KL expansion are smaller than the ones of the EOLE in the interior of the domain. However, the KL errors are larger than the EOLE error at the boundaries of the discretization domain. Li and Der Kiureghian (1993) observed the same for the KL and EOLE of univariate fields.

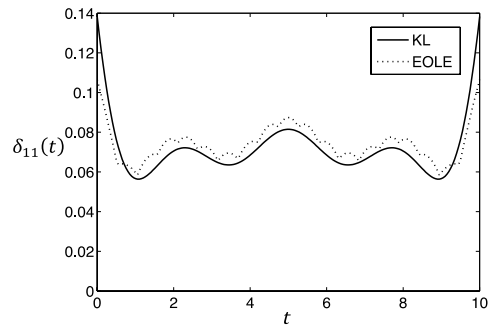

Figure 1. Point-wise variance error $\delta_{11}(t)$ for the multivariate KL and EOLE methods with $m = 6$.

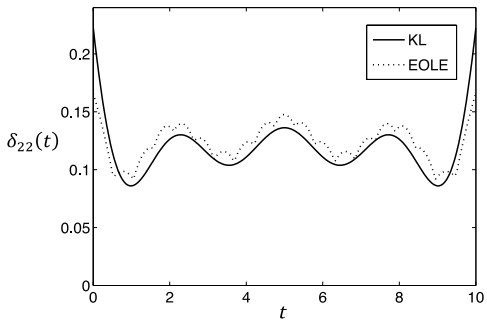

Figure 2. Point-wise variance error $\delta_{22}(t)$ for the multivariate KL and EOLE methods with $m = 6$.

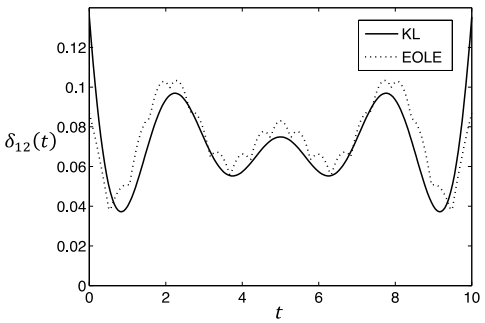

Figure 3. Point-wise covariance $\delta_{12}(t)$ of the discretization error of each component field for the multivariate KL and EOLE methods with $m = 6$.

Figure 4 shows the average errors of Eq. (4) against the number of random variables in the expansion for the multivariate EOLE. It is shown that the two variance errors $\bar{\delta}_{11}$ and $\bar{\delta}_{22}$ decrease monotonically with increase of the number of terms in the expansion. However, the same does not hold for the average covariance of the errors $\bar{\delta}_{12}$. This is due to the fact that the spatial functions of the EOLE representation are determined by minimizing the point-wise sum of the variance errors, i.e. the trace of $\boldsymbol{\Sigma}_{\boldsymbol{\epsilon}}(\mathbf{t})$, and not the covariance of the errors. As expected, the variance error of the component of the random field with the largest correlation length $\bar{\delta}_{11}$ is smaller than the one of the second component $\bar{\delta}_{22}$ at any order of expansion.

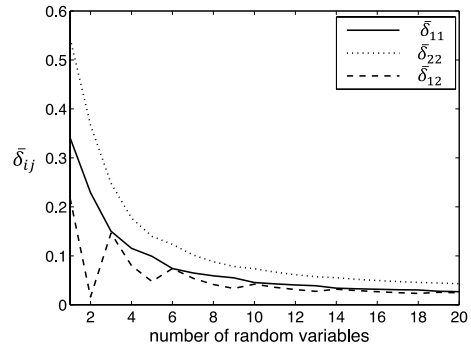

Figure 4. Average errors against number of random variables for the multivariate EOLE.

Figure 5 shows the sum of the average variance errors against the number of random variables in the expansion for the multivariate KL and EOLE methods. It is shown that the KL expansion has lower sum of variance errors than the EOLE. This is because the KL eigenfunctions minimize the sum of variance errors, relative to any orthogonal function set in $L^2(\Omega, \mathbb{R}^n)$.

Figure 6 compares the accuracy of the multivariate EOLE with the one of two correlated univariate EOLE expansions (corrEOLE). It is shown that the EOLE performs better than corrEOLE at any number of random variables in the representation. This is because in corrEOLE, each univariate EOLE representation is determined by minimizing the point-wise variance error of the corresponding random field. That is, the accuracy of the expansion depends on the autocorrelation functions of the two random fields, while their cross-correlation function is not considered. On the other hand, the spatial functions of the multivariate EOLE representation are found by minimizing the sum of variances of the two component random fields, which allows accounting for their cross-correlation. This is clearly seen in Eq. (44), wherein the matrix function $\boldsymbol{\Sigma}_q(\mathbf{t})$ expresses the covariance matrix function of the random field evaluated at a set of points.

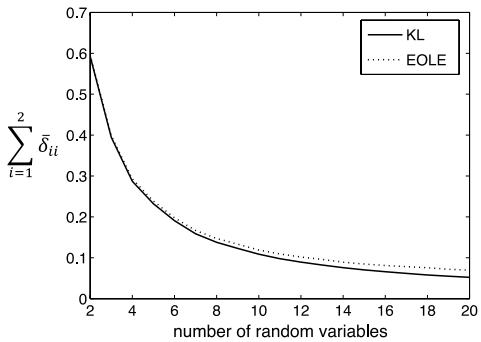

Figure 5. Sum of variance errors against number of random variables for the multivariate KL and EOLE methods.

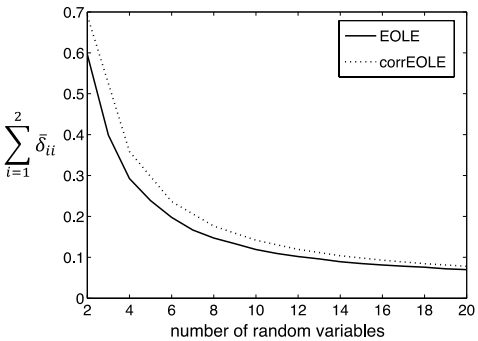

Figure 6. Sum of variance errors against number of random variables for the multivariate EOLE and for two correlated EOLE representations.

8 Conclusion

This paper reviewed series expansion methods for discretization of multivariate random fields and proposed a new method, namely the extension of EOLE to multivariate fields. The method is based on linear estimation theory for interpolation of dependent spatial data, i.e. the so-called co-kriging method. It was shown that the EOLE can be viewed as a numerical multivariate KL expansion. We also discussed the discretization of multivariate random fields with correlated univariate EOLE representations. It was shown that the multivariate EOLE is more efficient than correlated univariate EOLE representations because it accounts for the cross-correlation function of the random field in determining the spatial functions in the expansion.

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