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Reduced Chaos decomposition with random coefficients of vector-valued random variables and random fields

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ABSTRACT

We develop a stochastic functional representation that is adapted to problems involving various forms of epistemic uncertainties including modeling error and data paucity. The new representation builds on the polynomial Chaos decomposition and eventually yields a Karhunen–Loeve expansion with random multiplicative coefficients. In this expansion, one set of uncertainty is captured in the usual manner, as uncorrelated scalar random variables. Another component of the uncertainty, statistically independent from the first, is captured by constructing the, usually deterministic, functions in the KL expansion as random functions. We think of the first set of uncertainties as associated with a coarse scale model, and of the second set as associated with subscale fluctuations not captured in the coarse scale description.

1. Introduction

A number of challenges remain on the path to achieving the impact of stochastic analysis for the treatment of complex systems whose behavior is subject to uncertainties. These challenges can be broadly classified into three groups: Modeling, characterization, and propagation. In the modeling area, two further classifications can be identified. The first classification delineates between parametric and non-parametric interpretations of uncertainty. In the first case, uncertainty is attributed to stochastic fluctuations in the parameters of a physical model [11,21]. These fluctuations are typically interpreted as representing subscale fluctuations not fully resolved on the scale at which the governing physics is assumed to govern. In the second case, uncertainty is attributed to fluctuations in the form of the governing equations, leading to stochastic operator perturbations [19,20,5]. The second classification depends on the representative properties of the solution. Specifically, computed solutions can be representative of target solutions either in a distributional sense, a functional (L^2) sense, or an almost-sure sense, with distinct sets of mathematical tools applicable depending on the case. More specifically, approximation accuracy, model reduction, and the ingredients of a well-posed problem should all be defined in the context of what is meant by equality (distributional, in-the-norm, or almost-sure) [1]. We note that stochastic L^2 representations provide a characterization of the solution of a given problem as a deterministic functional form in terms of the stochastic parameters. This form for the solution is significant if sensitivity information and L^2-style error analysis are subsequently required, but otherwise seems to provide too much information. Likewise, a distributional equivalence between the computed solution and the exact solution is suitable if the details of the stochastic degrees of freedom (i.e. stochastic dimensions) are not relevant to the final analysis. The most significant challenge associated with characterizing uncertainty consists in faithfully capturing the weight of available evidence, with error analysis capabilities to determine the value of additional evidence. Methods for characterizing uncertainty are typically adapted to specific modeling approaches and rely on methods of statistical analysis including statistical estimation and statistical inference. Procedures based on maximum likelihood [12,6,9], Bayesian inference [10], and maximum entropy [4,19] have been put in place to characterize mathematical models based on polynomial Chaos decompositions and random matrix theory. The last challenge identified above relates to propagating uncertainty from data to predictions. This challenge has specific attributes depending on the interpretation of stochastic equality and on the specific stochastic model used. In all cases, however, it can be expected that the computational cost associated with this propagation step will grow with the complexity of the underlying stochastic data (requiring more stochastic degrees of freedom for a suitable characterization) and with the level of stochastic scatter in this data, typically resulting in a greater scatter in the predicted quantities of interest and a stronger nonlinear dependence of the predictions on the data.

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Significant progress has been achieved in recent years in the analysis of stochastic partial differential equations with random coefficients. In particular, theory and algorithms underlying polynomial Chaos and other functional approximation and projection methods have been set on firmer ground, providing a path forward towards a general purpose formulation of stochastic computational analysis [8,23,14,13,3,15,7,2,22,16]. Also, procedures for characterization and calibration of stochastic representations have been developed [12,6,10,9,4] that are well-adapted to functional approximation methods and their significance to model validation has been demonstrated [9]. Most of these developments have been with a view to either calibrating probabilistic models or accelerating the convergence of uncertainty propagation procedures, including methodologies for a-priori and a-posteriori error estimation. Modeling efforts that address the curse of dimensionality for complex uncertainties and that provide a framework for integrating epistemic uncertainty into the same unified framework as other sources of uncertainty have only recently begun to emerge While a number of efforts have introduced polynomial Chaos expansions where both the basis functions and their associated coordinates are random [17,10,9]. In these approaches, the mathematical analysis of these representations is still at a very fundamental level [18] that lags behind the nuances and sophistication of current practical needs. The present paper addresses this issue from a perspective that highlights its significance to problems of conceptual and mathematical modeling, calibration of probabilistic models, and computational efficiency. Specifically, we demonstrate how subset of the stochastic degrees of freedom can be rolled into the coefficients of a polynomial Chaos expansion, thus permitting the segregation of the uncertainties for subsequent processing. For example, the uncertainties that are retained for functional approximation can be treated using stochastic Galerkin projections, while the uncertainties that have been rolled into the coefficients can be treated using distributional representation. This hybrid treatment of uncertainties will adapt the computational effort and algorithms to the specific needs of the problem at hand. The final byproduct of our analysis is a Karhunen–Loeve decomposition where the, usually deterministic, coordinate functions are now themselves stochastic, endowed with a probabilistic measure that is independent of the measure associated with the standard orthogonal Karhunen–Loeve random variables.

In a first part of the paper, we show how the reduced Chaos decomposition with random coefficients of a $\mathbb{R}^n$-valued second-order random variable can be constructed and explore the mathematical properties of such a representation. A second part deals with the case of random fields. In the third part, we demonstrate our construction on an example that highlights some of its salient features.

2. Reduced Chaos decomposition with random coefficients of a vector-valued second-order random variable

2.1. Chaos decomposition of a vector-valued second-order random variable on a tensor product of two Hilbert spaces

In this subsection, we introduce the Chaos decomposition of a $\mathbb{R}^n$-valued second-order random variable with respect to the tensor product of two Hilbert spaces. This is a particular case of the more general setting analyzed in [21].

Let $\boldsymbol{X} = (X_1, \ldots, X_n)$, $\boldsymbol{Y} = (Y_1, \ldots, Y_m)$ and $\boldsymbol{Z} = (Z_1, \ldots, Z_p)$ be three second-order random variables, defined on a probability space $(\Theta, \mathcal{T}, P)$, with values in $\mathbb{R}^n$, $\mathbb{R}^m$ and $\mathbb{R}^p$, respectively. The probability distributions on $\mathbb{R}^n$ and $\mathbb{R}^m$ of random variables $\boldsymbol{X}$ and $\boldsymbol{Y}$ are assumed to be given and are denoted by $P_{\boldsymbol{X}}(d\boldsymbol{x})$ and $P_{\boldsymbol{Y}}(d\boldsymbol{y})$, in which $d\boldsymbol{x} = dx_1 \cdots dx_n$ and $d\boldsymbol{y} = dy_1 \cdots dy_m$ are the Lebesgue measures on $\mathbb{R}^n$ and $\mathbb{R}^m$. It is assumed that random variables $\boldsymbol{X}$ and $\boldsymbol{Y}$ are independent. Consequently, the joint probability distribution on $\mathbb{R}^n \times \mathbb{R}^m$ of random variables $\boldsymbol{X}$ and $\boldsymbol{Y}$ is written as $P_{\boldsymbol{X},\boldsymbol{Y}}(d\boldsymbol{x}, d\boldsymbol{y}) = P_{\boldsymbol{X}}(d\boldsymbol{x}) \otimes P_{\boldsymbol{Y}}(d\boldsymbol{y})$.

The random variable $\boldsymbol{Z}$ is assumed to be the transformation of $\boldsymbol{X}$ and $\boldsymbol{Y}$ by a measurable nonlinear mapping $(\boldsymbol{x}, \boldsymbol{y}) \mapsto \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y}) = (f_1(\boldsymbol{x}, \boldsymbol{y}), \ldots, f_p(\boldsymbol{x}, \boldsymbol{y}))$ from $\mathbb{R}^n \times \mathbb{R}^m$ into $\mathbb{R}^p$, in which $\boldsymbol{x} = (x_1, \ldots, x_n)$ and $\boldsymbol{y} = (y_1, \ldots, y_m)$. We then have $\boldsymbol{Z} = \boldsymbol{f}(\boldsymbol{X}, \boldsymbol{Y})$.

Since $\boldsymbol{f}$ is such that $\boldsymbol{Z}$ is a second-order random variable, we have

$$E\left\{\|\boldsymbol{f}(\boldsymbol{X}, \boldsymbol{Y})\|^2_{\mathbb{R}^p}\right\} = \int_{\mathbb{R}^n} \int_{\mathbb{R}^m} \|\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y})\|^2_{\mathbb{R}^p} P_{\boldsymbol{X},\boldsymbol{Y}}(d\boldsymbol{x}, d\boldsymbol{y}) < +\infty \tag{1}$$

in which $E\{\cdot\}$ denotes the mathematical expectation, and where $\|\cdot\|_{\mathbb{R}^p}$ denotes the Euclidean norm in $\mathbb{R}^p$ associated with the inner product $\langle \boldsymbol{z}, \boldsymbol{z}' \rangle_{\mathbb{R}^p} = z_1 z'_1 + \cdots + z_p z'_p$. From Eq. (1), it can be deduced that mapping $\boldsymbol{f}$ belongs to the space $L^2_{P_{\boldsymbol{X},\boldsymbol{Y}}}(\mathbb{R}^n \times \mathbb{R}^m, \mathbb{R}^p)$ of $P_{\boldsymbol{X},\boldsymbol{Y}}$-square-integrable functions from vector space $\mathbb{R}^n \times \mathbb{R}^m$ into vector space $\mathbb{R}^p$.

Let $\mathbb{H}_X = L^2_{P_{\boldsymbol{X}}}(\mathbb{R}^n)$ (resp. $\mathbb{H}_Y = L^2_{P_{\boldsymbol{Y}}}(\mathbb{R}^m)$) be the real Hilbert space of $P_{\boldsymbol{X}}$-square-integrable functions (resp. $P_{\boldsymbol{Y}}$-square-integrable functions) from vector space $\mathbb{R}^n$ (resp. $\mathbb{R}^m$) into $\mathbb{R}$. The real Hilbert spaces $\mathbb{H}_X$ and $\mathbb{H}_Y$ are equipped with the following inner products:

$$\langle u, u' \rangle_{\mathbb{H}_X} = \int_{\mathbb{R}^n} u(\boldsymbol{x}) u'(\boldsymbol{x}) P_{\boldsymbol{X}}(d\boldsymbol{x}) = E\{u(\boldsymbol{X}) u'(\boldsymbol{X})\}, \tag{2}$$

$$\langle v, v' \rangle_{\mathbb{H}_Y} = \int_{\mathbb{R}^m} v(\boldsymbol{y}) v'(\boldsymbol{y}) P_{\boldsymbol{Y}}(d\boldsymbol{y}) = E\{v(\boldsymbol{Y}) v'(\boldsymbol{Y})\}. \tag{3}$$

We introduce the multi-index $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$ and the multi-index $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_m) \in \mathbb{N}^m$. Let us consider a Hilbertian basis of real Hilbert space $\mathbb{H}_X$ (resp. $\mathbb{H}_Y$) given by $\{\varphi_{\boldsymbol{\alpha}}, \boldsymbol{\alpha} \in \mathbb{N}^n\}$ (resp. $\{\psi_{\boldsymbol{\beta}}, \boldsymbol{\beta} \in \mathbb{N}^m\}$). We thus have

$$\langle \varphi_{\boldsymbol{\alpha}}, \varphi_{\boldsymbol{\alpha}'} \rangle_{\mathbb{H}_X} = E\{\varphi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \varphi_{\boldsymbol{\alpha}'}(\boldsymbol{X})\} = \delta_{\boldsymbol{\alpha}\boldsymbol{\alpha}'}, \tag{4}$$

$$\langle \psi_{\boldsymbol{\beta}}, \psi_{\boldsymbol{\beta}'} \rangle_{\mathbb{H}_Y} = E\{\psi_{\boldsymbol{\beta}}(\boldsymbol{Y}) \psi_{\boldsymbol{\beta}'}(\boldsymbol{Y})\} = \delta_{\boldsymbol{\beta}\boldsymbol{\beta}'}. \tag{5}$$

Therefore, any function $g \in \mathbb{H}_X$ (resp. $h \in \mathbb{H}_Y$) can be expanded as

$$g(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^n} g_{\boldsymbol{\alpha}} \varphi_{\boldsymbol{\alpha}}(\boldsymbol{x}), \quad h(\boldsymbol{y}) = \sum_{\boldsymbol{\beta} \in \mathbb{N}^m} h_{\boldsymbol{\beta}} \psi_{\boldsymbol{\beta}}(\boldsymbol{y}) \tag{6}$$

in which

$$g_{\boldsymbol{\alpha}} = \langle g, \varphi_{\boldsymbol{\alpha}} \rangle_{\mathbb{H}_X} = E\{g(\boldsymbol{X}) \; \varphi_{\boldsymbol{\alpha}}(\boldsymbol{X})\}, \quad h_{\boldsymbol{\beta}} = \langle h, \psi_{\boldsymbol{\beta}} \rangle_{\mathbb{H}_Y} = E\{h(\boldsymbol{Y}) \; \psi_{\boldsymbol{\beta}}(\boldsymbol{Y})\}. \tag{7}$$

Below, it is assumed that the Hilbertian bases $\varphi_{\boldsymbol{\alpha}}$ and $\psi_{\boldsymbol{\beta}}$ are polynomial bases such that

$$\varphi_{\boldsymbol{0}}(\boldsymbol{X}) = 1, \quad \psi_{\boldsymbol{0}}(\boldsymbol{Y}) = 1. \tag{8}$$

Consequently, we deduce that

$$E\{\varphi_{\boldsymbol{\alpha}}(\boldsymbol{X})\} = 0, \quad \forall \boldsymbol{\alpha} \neq \boldsymbol{0} \quad \text{and} \quad E\{\psi_{\boldsymbol{\beta}}(\boldsymbol{Y})\} = 0, \quad \forall \boldsymbol{\beta} \neq \boldsymbol{0}. \tag{9}$$

It can then be proven [21] that the $\mathbb{R}^p$-valued random variable $\boldsymbol{Z} = \boldsymbol{f}(\boldsymbol{X}, \boldsymbol{Y})$ has the following Chaos representation related to the tensor product of $\mathbb{H}_X$ with $\mathbb{H}_Y$,

$$\boldsymbol{Z} = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^n} \sum_{\boldsymbol{\beta} \in \mathbb{N}^m} \boldsymbol{z}^{\boldsymbol{\alpha}\boldsymbol{\beta}} \varphi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \psi_{\boldsymbol{\beta}}(\boldsymbol{Y}) \tag{10}$$

in which the coefficients $\boldsymbol{z}^{\boldsymbol{\alpha}\boldsymbol{\beta}} \in \mathbb{R}^p$ are given by

$$\boldsymbol{z}^{\boldsymbol{\alpha}\boldsymbol{\beta}} = E\{\boldsymbol{Z} \varphi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \psi_{\boldsymbol{\beta}}(\boldsymbol{Y})\}. \tag{11}$$

We then have the following properties concerning the second-order moments of random variable $\boldsymbol{Z}$,