# A polynomial chaos expansion in dependent random variables ${ }^{\text {*T }}$ 

Sharif Rahman<br>Applied Mathematical and Computational Sciences, The University of Iowa, Iowa City, IA 52242, USA

## A R T I C L E IN F O

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#### Abstract

This paper introduces a new generalized polynomial chaos expansion (PCE) comprising measure-consistent multivariate orthonormal polynomials in dependent random variables. Unlike existing PCEs, whether classical or generalized, no tensorproduct structure is assumed or required. Important mathematical properties of the generalized PCE are studied by constructing orthogonal decomposition of polynomial spaces, explaining completeness of orthogonal polynomials for prescribed assumptions, exploiting whitening transformation for generating orthonormal polynomial bases, and demonstrating mean-square convergence to the correct limit. Analytical formulae are proposed to calculate the mean and variance of a truncated generalized PCE for a general output variable in terms of the expansion coefficients. An example derived from a stochastic boundary-value problem illustrates the generalized PCE approximation in estimating the statistical properties of an output variable for 12 distinct non-product-type probability measures of input variables.


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## 1. Introduction

Polynomial chaos expansion (PCE) is an infinite series expansion of an output random variable involving orthogonal polynomials in input random variables. Introduced by Wiener [22] for Gaussian input variables, followed by a proof of convergence [2], the original PCE, referred to as the classical PCE in this paper, was later extended to a generalized PCE [23] to account for non-Gaussian variables. Approximations derived from truncated PCE, whether classical or generalized, are commonly used for solving uncertainty quantification problems, mostly in the context of solving stochastic partial differential equations [11,21], yielding approximate second-moment statistics of an output random variable of interest. However, the existing PCE is largely founded on the independence assumption of input variables. The assumption exploits product-type probability measures, facilitating construction of the space of multivariate orthogonal polynomials via tensor product of the spaces of univariate orthogonal polynomials. In reality, there may exist significant correlation or dependence among input variables, impeding or invalidating many stochastic methods, including PCE.

[^0]The Rosenblatt transformation [18], commonly used for mapping dependent to independent variables, may induce very strong nonlinearity to a stochastic response, potentially degrading or even prohibiting convergence of probabilistic solutions [16]. While the works of Soize and Ghanem [20] and Rahman [17] to cope with dependent variables are a step in the right direction, they, respectively, employ non-polynomial basis unamenable to producing analytical formulae for response statistics and focus strictly on Gaussian variables. Furthermore, the first of these studies does not address denseness or completeness of basis functions or account for infinitely many input variables. Therefore, innovations beyond tensor-product PCEs, capable of tackling non-product-type probability measures, are highly desirable.

This study delves into a number of mathematical issues concerning necessary and sufficient conditions for the completeness of multivariate orthogonal polynomials; convergence, exactness, and optimal analyses; and approximation quality due to truncation - all associated with a generalized PCE for dependent, non-product-type probability measures. Therefore, the results of this paper are new in many aspects. The paper is organized as follows. Section 2 defines or discusses mathematical notations and preliminaries. A set of assumptions on the input probability measure required by the generalized PCE is explained. A brief exposition of multivariate orthogonal polynomials consistent with a general, non-product-type probability measure, including their second moment properties, is given in Section 3. The section also describes relevant polynomial spaces and construction of their orthogonal decompositions. The orthogonal basis and completeness of multivariate orthogonal polynomials have also been established. Section 4 defines the polynomial moment matrix, resulting in a variety of whitening transformations to produce measure-consistent orthonormal polynomials. The statistical properties of both orthogonal and orthonormal polynomials are presented. Section 5 formally introduces the generalized PCE for a square-integrable random variable. The convergence, exactness, and optimality of the generalized PCE are explained. In the same section, the approximation quality of a truncated generalized PCE is discussed. The formulae for the mean and variance of a truncated generalized PCE are derived, and methods for estimating the expansion coefficients are outlined. The section ends with an explanation on how and when the generalized PCE proposed can be extended for infinitely many input variables. The results from a simple yet illuminating example are reported in Section 6 with supplementary details in Appendix A. Finally, conclusions are drawn in Section 7.

## 2. Input random variables

Let $\mathbb{N}:=\{1,2, \ldots\}, \mathbb{N}_{0}:=\mathbb{N} \cup\{0\}, \mathbb{R}:=(-\infty,+\infty)$, and $\mathbb{R}_{0}^{+}:=[0,+\infty)$ represent the sets of positive integer (natural), non-negative integer, real, and non-negative real numbers, respectively. For a non-zero, finite integer $N \in \mathbb{N}$, denote by $\mathbb{A}^{N} \subseteq \mathbb{R}^{N}$ a bounded or unbounded subdomain of $\mathbb{R}^{N}$. The set of $N \times N$ real-valued square matrices is denoted by $\mathbb{R}^{N \times N}$.

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a complete probability space, where $\Omega$ is a sample space representing an abstract set of elementary events, $\mathcal{F}$ is a $\sigma$-algebra on $\Omega$, and $\mathbb{P}: \mathcal{F} \rightarrow[0,1]$ is a probability measure. With $\mathcal{B}^{N}:=$ $\mathcal{B}\left(\mathbb{A}^{N}\right)$ representing the Borel $\sigma$-algebra on $\mathbb{A}^{N} \subseteq \mathbb{R}^{N}$, consider an $\mathbb{A}^{N}$-valued input random vector $\mathbf{X}:=$ $\left(X_{1}, \ldots, X_{N}\right)^{T}:(\Omega, \mathcal{F}) \rightarrow\left(\mathbb{A}^{N}, \mathcal{B}^{N}\right)$, describing the statistical uncertainties in all system parameters of a stochastic problem. The input random variables are also referred to as basic random variables. The integer $N$ represents the number of input random variables and is referred to as the dimension of the stochastic problem.

Denote by $F_{\mathbf{X}}(\mathbf{x}):=\mathbb{P}\left(\cap_{i=1}^{N}\left\{X_{i} \leq x_{i}\right\}\right)$ the joint distribution function of $\mathbf{X}$, admitting the joint probability density function $f_{\mathbf{X}}(\mathbf{x}):=\partial^{N} F_{\mathbf{X}}(\mathbf{x}) / \partial x_{1} \cdots \partial x_{N}$. Given the abstract probability space $(\Omega, \mathcal{F}, \mathbb{P})$, the image probability space is $\left(\mathbb{A}^{N}, \mathcal{B}^{N}, f_{\mathbf{X}} d \mathbf{x}\right)$, where $\mathbb{A}^{N}$ can be viewed as the image of $\Omega$ from the mapping $\mathbf{X}: \Omega \rightarrow \mathbb{A}^{N}$, and is also the support of $f_{\mathbf{X}}(\mathbf{x})$. Relevant statements and objects in one space have obvious counterparts in the other space. Both probability spaces will be used in this paper.

A set of assumptions used or required by the generalized PCE is as follows.

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    E-mail address: sharif-rahman@uiowa.edu.

