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Uncertainty quantification under dependent random variables by a generalized polynomial dimensional decomposition☆

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Abstract

This paper is concerned with uncertainty quantification analysis of complex systems subject to dependent input random variables. The analysis focuses on a new, generalized version of polynomial dimensional decomposition (PDD), referred to as GPDD, entailing hierarchically ordered measure-consistent multivariate orthogonal polynomials in dependent variables. Under a few prescribed assumptions, GPDD exists for any square-integrable output random variable and converges in mean-square to the correct limit. New analytical formulae are proposed to calculate the mean and variance of a GPDD approximation of a general output variable in terms of the expansion coefficients and second-moment properties of multivariate orthogonal polynomials. However, unlike in PDD, calculating the coefficients of GPDD requires solving a coupled system of linear equations. Besides, the variance formula of GPDD contains extra terms due to statistical dependence among input variables. The extra terms disappear when the input variables are statistically independent, reverting GPDD to PDD. Two numerical examples, the one derived from a stochastic boundary-value problem and the other entailing a random eigenvalue problem, illustrate second-moment error analysis and estimation of the probabilistic characteristics of eigensolutions.

Keywords: ANOVA; Multivariate orthogonal polynomials; Non-product-type probability measures

1. Introduction

Uncertainty quantification (UQ) in computational models of complex systems is a crucial ingredient in numerous fields of science and engineering as diverse as climate science, mechanics, material science, finance, and medicine. In practice, confronting hundreds of input variables or more is no longer unusual, where a response variable of interest, defined algorithmically via time-consuming finite-element analysis (FEA) or similar numerical calculations, is all too often costly to evaluate. Contemporary surrogate methods or approximations, for instance, stochastic collocation [1,2], polynomial chaos expansion (PCE) [3,4], and sparse-grid approximation [5,6], are known to impart

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hefty computational benefit over crude Monte Carlo simulation (MCS). However, for truly high-dimensional systems, they require astronomically large numbers of terms or coefficients, thereby acceding to the curse of dimensionality. Therefore, alternative computational methods capitalizing on low effective dimensions [7] of high-dimensional functions, such as the polynomial dimensional decomposition (PDD) methods [8–10], are desirable. Although PDD and PCE are built using the same measure-consistent orthogonal polynomials, a recent mathematical study reveals that PDD cannot commit larger error than PCE for identical expansion orders [11]. Moreover, to estimate with the same precision the variance of an output function involving exponentially attenuating expansion coefficients, the PDD approximation can be markedly more efficient than the PCE approximation.

However, the success of PDD is largely predicated on the independent assumption of input random variables, because the analysis-of-variance (ANOVA) dimensional decomposition (ADD) [12–16], which leads to PDD, is fundamentally rooted in the product structure of the probability distribution. In reality, there may exist significant correlation or dependence among input variables, hindering or invalidating most existing stochastic methods, including PDD. Indeed, ignoring these correlations or dependencies, whether emanating from loads, material properties, or manufacturing variables, may produce inaccurate or inadequate designs [17]. Therefore, the classical ADD and existing PDD must be generalized for an arbitrary, non-product-type probability measure. Doing so will require modifying the foundations of the classical ADD that will endow desirable stochastic properties of PDD, insofar as is possible, to the generalization. Such capabilities are currently lacking, but are critical for paradigm-shifting advances in UQ theory and praxis.

The main objective of this study is to create a new, generalized version of PDD, referred to as GPDD, for UQ analysis of complex systems in the presence of arbitrary, dependent probability measures of input variables. While this paper focuses on the computational aspect of the generalization, readers interested in a rigorous mathematical analysis of GPDD, including theoretical results and their formal proofs, should consult the companion paper [18]. The paper is organized as follows. Section 2 discusses mathematical notations and preliminaries, including a list of four requisite assumptions. A brief exposition of multivariate orthogonal polynomials consistent with a general, non-product-type probability measure, including their statistical properties, is given in Section 3. The orthogonal basis and completeness of multivariate orthogonal polynomials have been established. In this section and Appendix A, a special class of orthogonal polynomials generated from the derivatives of the probability density functions is also discussed. Section 4 introduces GPDD for a square-integrable output random variable, including the approximation or method emanating from a truncated GPDD. In the same section, new analytical formulae for the mean and variance of a truncated GPDD are derived. An algorithm for numerical implementation of the GPDD method is outlined. The GPDD results of second-moment error analysis obtained for a stochastic ordinary differential equation (ODE) are reported in Section 5 with supplementary details in Appendix B. The section also demonstrates an engineering application of GPDD by estimating the probabilistic characteristics of random eigensolutions from structural dynamics. Section 6 discusses a few computational challenges for future work. Finally, conclusions are drawn in Section 7.

2. Notation, preliminaries, and assumptions

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 $\mathbb{R}^N$.

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a complete probability space, where Ω is a sample space representing an abstract set of elementary events, $\mathcal{F}$ is a σ-algebra on Ω, and $\mathbb{P} : \mathcal{F} \to [0, 1]$ is a probability measure. With $\mathcal{B}^N := \mathcal{B}(\mathbb{A}^N)$ representing the Borel σ-algebra on $\mathbb{A}^N \subseteq \mathbb{R}^N$, consider an $\mathbb{A}^N$-valued input random vector $\mathbf{X} := (X_1, \ldots, X_N)^T : (\Omega, \mathcal{F}) \to (\mathbb{A}^N, \mathcal{B}^N)$, describing the statistical uncertainties in all system parameters of a UQ problem. The input random variables are generally dependent and are also referred to as basic random variables. The integer N represents the number of input random variables and is often referred to as the dimension of the UQ problem.

Denote by $F_{\mathbf{X}}(\mathbf{x}) := \mathbb{P}(\cap_{i=1}^N \{X_i \le x_i\})$ 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 $(\mathbb{A}^N, \mathcal{B}^N, f_{\mathbf{X}} d\mathbf{x})$, where $\mathbb{A}^N$ can be viewed as the image of Ω from the mapping $\mathbf{X} : \Omega \to \mathbb{A}^N$, and is also the support of $f_{\mathbf{X}}(\mathbf{x})$.

It is assumed that the random vector $\mathbf{X} := (X_1, \ldots, X_N)^T : (\Omega, \mathcal{F}) \to (\mathbb{A}^N, \mathcal{B}^N)$ has

(1) an absolutely continuous joint distribution function $F_{\mathbf{X}}(\mathbf{x})$ and a continuous joint probability density function $f_{\mathbf{X}}(\mathbf{x})$ with a bounded or unbounded support $\mathbb{A}^N$;

(2) absolute finite moments of all orders, that is, for all $\mathbf{j} := (j_1, \ldots, j_N) \in \mathbb{N}_0^N$,

$$\mathbb{E}[|\mathbf{X}^{\mathbf{j}}|] < \infty,$$

where $\mathbf{X}^{\mathbf{j}} = X_1^{j_1} \cdots X_N^{j_N}$ and $\mathbb{E}$ is the expectation operator with respect to the probability measure $\mathbb{P}$ or $f_{\mathbf{X}}(\mathbf{x})d\mathbf{x}$;

(3) a joint probability density function $f_{\mathbf{X}}(\mathbf{x})$, which is either (a) compactly supported or (b) exponentially integrable, that is, there exists a real number $a > 0$ such that

$$\mathbb{E}[\exp(a\|\mathbf{X}\|)] < \infty,$$

where $\|\cdot\| : \mathbb{A}^N \to \mathbb{R}_0^+$ is an arbitrary norm; and

(4) a joint probability density function $f_{\mathbf{X}}(\mathbf{x})$ with a grid-closed support, that is, there exists a grid for every point $\mathbf{x}$ of $\text{supp}(f_{\mathbf{X}}) = \mathbb{A}^N \subseteq \mathbb{R}^N$.

Unless otherwise stated, all four assumptions are employed throughout the paper.

3. Multivariate orthogonal polynomials

For $N \in \mathbb{N}$, denote by $\{1, \ldots, N\}$ an index set, so that $u \subseteq \{1, \ldots, N\}$ is a subset, including the empty set $\emptyset$, with cardinality $0 \le |u| \le N$. The complementary subset of u is denoted by $-u := \{1, \ldots, N\} \setminus u$. For $\emptyset \ne u \subseteq \{1, \ldots, N\}$, let $\mathbf{X}_u := (X_{i_1}, \ldots, X_{i_{|u|}})^T$, $1 \le i_1 < \cdots < i_{|u|} \le N$, a subvector of $\mathbf{X}$, be defined on the abstract probability space $(\Omega^u, \mathcal{F}^u, \mathbb{P}^u)$, where Ω^u is the sample space of $\mathbf{X}_u$, $\mathcal{F}^u$ is a σ-algebra on Ω^u, and $\mathbb{P}^u$ is a probability measure. The complementary subvector is defined by $\mathbf{X}_{-u} := \mathbf{X}_{\{1,\ldots,N\}\setminus u}$. The corresponding image probability space is $(\mathbb{A}^u, \mathcal{B}^u, f_{\mathbf{X}_u}d\mathbf{x}_u)$, where $\mathbb{A}^u \subseteq \mathbb{R}^{|u|}$ is the image sample space of $\mathbf{X}_u$, $\mathcal{B}^u$ is the Borel σ-algebra on $\mathbb{A}^u$, and $f_{\mathbf{X}_u}(\mathbf{x}_u) := \int_{\mathbb{A}^{-u}} f_{\mathbf{X}}(\mathbf{x})d\mathbf{x}_{-u}$ is the marginal probability density function of $\mathbf{X}_u$ supported on $\mathbb{A}^u$.

Let $\mathbf{X}$ be an input random vector with a general probability measure $f_{\mathbf{X}}(\mathbf{x})d\mathbf{x}$ on $\mathbb{A}^N$, satisfying Assumptions (1)–(3). When $\emptyset \ne u \subseteq \{1, \ldots, N\}$, a $|u|$-dimensional multi-index is denoted by $\mathbf{j}_u := (j_{i_1}, \ldots, j_{i_{|u|}}) \in \mathbb{N}_0^{|u|}$ with the total degree $|\mathbf{j}_u| := j_{i_1} + \cdots + j_{i_{|u|}}$, where $j_{i_p} \in \mathbb{N}_0$, $p = 1, \ldots, |u|$, represents the pth component of $\mathbf{j}_u$.[2]

3.1. Measure-consistent orthogonal polynomials

Denote by

$$\Pi^u := \mathbb{R}[\mathbf{x}_u] = \mathbb{R}[x_{i_1}, \ldots, x_{i_{|u|}}]$$

the space of all real polynomials in $\mathbf{x}_u$. For any polynomial pair $P_u, Q_u \in \Pi^u$, $\emptyset \ne u \subseteq \{1, \ldots, N\}$, define an inner product

$$(P_u, Q_u)_{f_{\mathbf{X}_u}d\mathbf{x}_u} := \int_{\mathbb{A}^u} P_u(\mathbf{x}_u)Q_u(\mathbf{x}_u)f_{\mathbf{X}_u}(\mathbf{x}_u)d\mathbf{x}_u = \mathbb{E}\left[P_u(\mathbf{X}_u)Q_u(\mathbf{X}_u)\right] \tag{1}$$

on Π^u with respect to the measure $f_{\mathbf{X}_u}(\mathbf{x}_u)d\mathbf{x}_u$. The polynomials $P_u \in \Pi^u$ and $Q_u \in \Pi^u$ are called orthogonal to each other with respect to $f_{\mathbf{X}_u}(\mathbf{x}_u)d\mathbf{x}_u$ if $(P_u, Q_u)_{f_{\mathbf{X}_u}d\mathbf{x}_u} = 0$. Moreover, a polynomial $P_u \in \Pi^u$ is said to be an orthogonal polynomial with respect to $f_{\mathbf{X}_u}(\mathbf{x}_u)d\mathbf{x}_u$ if it is orthogonal to all polynomials of lower degree, that is, if [19]

$$(P_u, Q_u)_{f_{\mathbf{X}_u}d\mathbf{x}_u} = 0 \;\forall Q_u \in \Pi^u \text{ with } \deg Q_u < \deg P_u. \tag{2}$$

Under Assumptions (1) and (2), moments of $\mathbf{X}_u$ of all orders exist and are finite, so that the inner product in (1) is well defined. Then there exists an infinite set of multivariate orthogonal polynomials, say, $\{P_{u,\mathbf{j}_u}(\mathbf{x}_u) : \mathbf{j}_u \in \mathbb{N}_0^{|u|}\}$, $P_{u,\mathbf{0}} = 1$, $P_{u,\mathbf{j}_u} \ne 0$, which is consistent with the probability measure $f_{\mathbf{X}_u}(\mathbf{x}_u)d\mathbf{x}_u$, satisfying

$$\left(P_{u,\mathbf{j}_u}, P_{u,\mathbf{k}_u}\right)_{f_{\mathbf{X}_u}d\mathbf{x}_u} = 0 \text{ whenever } |\mathbf{j}_u| \ne |\mathbf{k}_u| \tag{3}$$

for $\mathbf{k}_u \in \mathbb{N}_0^{|u|}$. Here, the multi-index $\mathbf{j}_u$ of the multivariate polynomial $P_{u,\mathbf{j}_u}(\mathbf{x}_u)$ refers to its total degree $|\mathbf{j}_u|$. Clearly, each $P_{u,\mathbf{j}_u} \in \Pi^u$ is an orthogonal polynomial satisfying (2). This means that $P_{u,\mathbf{j}_u}$ is orthogonal to all polynomials of different degrees, but it may not be orthogonal to other orthogonal polynomials of the same degree.

[2] The same symbol $|\cdot|$ is used for designating both the cardinality of a set and the degree of a multi-index in this paper.

Perhaps the most commonly cited example of classical multivariate orthogonal polynomials is the case of multivariate Hermite polynomials, which are consistent with the measure defined by a Gaussian density [20,21]. Readers interested to learn more about orthogonal polynomials in multiple variables with respect to other measures are referred to the works of Appell and de Fériet [22], Erdélyi [20], Krall and Sheffer [23], and Dunkl and Xu [19].

For general probability measures, established numerical techniques, such as the Gram–Schmidt orthogonalization process [24], can be applied to a sequence of monomials $\{\mathbf{x}_u^{\mathbf{j}_u}\}_{\mathbf{j}_u \in \mathbb{N}_0^{|u|}}$ with respect to the inner product in (1) to generate a corresponding sequence of any measure-consistent orthogonal polynomials. However, it is important to emphasize that the space of multivariate orthogonal polynomials for a generally non-product-type density function cannot be constructed by the tensor product of the spaces of univariate orthogonal polynomials.

Once the multivariate orthogonal polynomials are obtained, they can be scaled to generate the standardized version of measure-consistent multivariate orthogonal polynomials

$$\Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) := \frac{P_{u,\mathbf{j}_u}(\mathbf{x}_u)}{\sqrt{\mathbb{E}[P^2_{u,\mathbf{j}_u}(\mathbf{X}_u)]}},\ \emptyset \neq u \subseteq \{1,\dots,N\},\ \mathbf{j}_u \in \mathbb{N}_0^{|u|}. \tag{4}$$

The standardization is not absolutely required, but it produces relatively simpler expressions of GPDD and subsequent results. The standardized polynomials are used in numerical examples.

3.2. Dimension-wise decomposition of polynomial spaces

A decomposition of polynomial spaces entailing dimension-wise splitting leads to GPDD. Here, to facilitate such splitting of the polynomial space Π^u for any $\emptyset \neq u \subseteq \{1,\dots,N\}$, limit the component j_{i_p} associated with the i_pth variable, where $i_p \in u \subseteq \{1,\dots,N\}$, $p = 1,\dots,|u|$, and $|u| > 0$, to take on only positive integer values. In consequence, $\mathbf{j}_u := (j_{i_1},\dots,j_{i_{|u|}}) \in \mathbb{N}^{|u|}$, the multi-index of $P_{u,\mathbf{j}_u}(\mathbf{x}_u)$, has degree $|\mathbf{j}_u| = j_{i_1} + \cdots + j_{i|u|}$, varying from $|u|$ to ∞ as $j_{i_1} \neq \cdots j_{i_{|u|}} \neq 0$.

For $\mathbf{j}_u \in \mathbb{N}^{|u|}$ and $\mathbf{x}_u := (x_{i_1},\dots,x_{i_{|u|}})$, a monomial in the variables $x_{i_1},\dots,x_{i_{|u|}}$ is the product $\mathbf{x}_u^{\mathbf{j}_u} = x_{i_1}^{j_{i_1}} \dots x_{i_{|u|}}^{j_{i_{|u|}}}$ and has a total degree $|\mathbf{j}_u|$. A linear combination of $\mathbf{x}_u^{\mathbf{j}_u}$, where $|\mathbf{j}_u| = l$, $|u| \leq l < \infty$, is a homogeneous polynomial in $\mathbf{x}_u$ of degree l. For $\emptyset \neq u \subseteq \{1,\dots,N\}$, denote by

$$\mathcal{Q}_l^u := \text{span}\{\mathbf{x}_u^{\mathbf{j}_u} : |\mathbf{j}_u| = l,\ \mathbf{j}_u \in \mathbb{N}^{|u|}\},\ |u| \leq l < \infty,$$

the space of homogeneous polynomials in $\mathbf{x}_u$ of degree l where the individual degree of each variable is non-zero and by

$$\Theta_m^u := \text{span}\{\mathbf{x}_u^{\mathbf{j}_u} : |u| \leq |\mathbf{j}_u| \leq m,\ \mathbf{j}_u \in \mathbb{N}^{|u|}\},\ |u| \leq m < \infty,$$

the space of polynomials in $\mathbf{x}_u$ of degree at least $|u|$ and at most m where the individual degree of each variable is non-zero.

Let $\mathcal{Z}_{|u|}^u := \Theta_{|u|}^u$. For each $|u| + 1 \leq l < \infty$, denote by $\mathcal{Z}_l^u \subset \Theta_l^u$ the space of orthogonal polynomials of degree exactly l that are orthogonal to all polynomials in Θ_{l-1}^u, that is,

$$\mathcal{Z}_l^u := \{P_u \in \Theta_l^u : (P_u, Q_u)_{f_{\mathbf{X}_u} d\mathbf{x}_u} = 0\ \forall\ Q_u \in \Theta_{l-1}^u\},\ |u| + 1 \leq l < \infty.$$

Then $\mathcal{Z}_l^u$, provided that the support of $f_{\mathbf{X}_u}(\mathbf{x}_u)$ has non-empty interior, is a vector space of dimension [18]

$$M_{u,l} := \dim \mathcal{Z}_l^u = \dim \mathcal{Q}_l^u = \binom{l-1}{|u|-1}.$$

Many choices exist for the basis of $\mathcal{Z}_l^u$. Here, as proved in the companion paper [18], $\{P_{u,\mathbf{j}_u}(\mathbf{x}_u) : |\mathbf{j}_u| = l, \mathbf{j}_u \in \mathbb{N}^{|u|}\} \subset \mathcal{Z}_l^u$ forms a basis of $\mathcal{Z}_l^u$, comprising $M_{u,l}$ number of basis functions. Each basis function $P_{u,\mathbf{j}_u}(\mathbf{x}_u)$ is a multivariate orthogonal polynomial of degree $|\mathbf{j}_u|$ as defined earlier. Clearly,

$$\mathcal{Z}_l^u = \text{span}\{P_{u,\mathbf{j}_u}(\mathbf{x}_u) : |\mathbf{j}_u| = l, \mathbf{j}_u \in \mathbb{N}^{|u|}\},\ |u| \leq l < \infty.$$

According to (3), $P_{u,\mathbf{j}_u}(\mathbf{X}_u)$ is orthogonal to $P_{u,\mathbf{k}_u}(\mathbf{X}_u)$ whenever $|\mathbf{j}_u| \neq |\mathbf{k}_u|$. Therefore, any two distinct polynomial subspaces $\mathcal{Z}_l^u$ and $\mathcal{Z}_{l'}^u$, where $\emptyset \neq u \subseteq \{1,\dots,N\}$, $|u| \leq l < \infty$, and $|u| \leq l' < \infty$, are orthogonal whenever $l \neq l'$.

Consequently, there exists a decomposition of

$$\begin{aligned} \mathit{\Pi}^N &= \mathbf{1} \oplus \bigcup_{\emptyset \neq u \subseteq \{1,\ldots,N\}} \bigoplus_{l=|u|}^{\infty} \mathcal{Z}_l^u \\ &= \mathbf{1} \oplus \bigcup_{\emptyset \neq u \subseteq \{1,\ldots,N\}} \bigoplus_{l=|u|}^{\infty} \text{span}\{P_{u,\mathbf{j}_u}(\mathbf{x}_u) : |\mathbf{j}_u| = l, \mathbf{j}_u \in \mathbb{N}^{|u|}\} \\ &= \mathbf{1} \oplus \bigcup_{\emptyset \neq u \subseteq \{1,\ldots,N\}} \text{span}\{P_{u,\mathbf{j}_u}(\mathbf{x}_u) : \mathbf{j}_u \in \mathbb{N}^{|u|}\}, \end{aligned}$$

where the symbol $\oplus$ represents the orthogonal sum of vector spaces and $\mathbf{1} := \text{span}\{1\}$, the constant subspace, needs to be added because the subspace $\mathcal{Z}_l^u$ excludes constant functions [18].

Given the dimension-wise splitting of $\mathit{\Pi}^N$, any square-integrable function of input random vector $\mathbf{X}$ can be expanded as a Fourier-like series of hierarchically ordered multivariate orthogonal polynomials in $\mathbf{X}_u$, $\emptyset \neq u \subseteq \{1, \ldots, N\}$. The expansion defines GPDD, to be formally presented in Section 4.

3.3. Completeness of orthogonal polynomials and basis

An important question regarding orthogonal polynomials is whether they are complete and constitute a basis in $L^2(\mathbb{A}^N, \mathcal{B}^N, f_{\mathbf{X}}d\mathbf{x})$, which represents the Hilbert space of square-integrable functions with respect to the probability measure $f_{\mathbf{X}}(\mathbf{x})d\mathbf{x}$ supported on $\mathbb{A}^N$. Under Assumptions (1)–(3), it can be shown that, indeed, these orthogonal polynomials span the Hilbert space of interest [18]. Therefore, the set of polynomials from the union-sum collection

$$\mathbf{1} \oplus \bigcup_{\emptyset \neq u \subseteq \{1,\ldots,N\}} \bigoplus_{l=|u|}^{\infty} \text{span}\{P_{u,\mathbf{j}_u}(\mathbf{x}_u) : |\mathbf{j}_u| = l, \mathbf{j}_u \in \mathbb{N}^{|u|}\}$$

is dense in $L^2(\mathbb{A}^N, \mathcal{B}^N, f_{\mathbf{X}}d\mathbf{x})$. The denseness or completeness is vitally important for the mean-square convergence of GPDD to the correct limit [18].

3.4. Statistical properties of random multivariate polynomials

When the input random variables $X_1, \ldots, X_N$, instead of real variables $x_1, \ldots, x_N$, are inserted in the argument, the multivariate polynomials $P_{u,\mathbf{j}_u}(\mathbf{X}_u)$ or $\Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)$, where $\emptyset \neq u \subseteq \{1, \ldots, N\}$ and $\mathbf{j}_u \in \mathbb{N}^{|u|}$, become functions of random input variables. Therefore, it is important to establish their second-moment properties, as follows.

3.4.1. Annihilating conditions

Under Assumptions (1)–(4), there exist weak annihilating conditions, which mandate that each polynomial of the set $\{P_{u,\mathbf{j}_u}(\mathbf{x}_u) : \mathbf{j}_u \in \mathbb{N}^N\}$ integrates to *zero* with respect to the marginal density function $f_{\mathbf{X}_u}(\mathbf{x}_u)$ of $\mathbf{X}_u$ in each coordinate direction of u, that is [18],

$$\int_{\mathbb{A}^{\{i\}}} P_{u,\mathbf{j}_u}(\mathbf{x}_u) f_{\mathbf{X}_u}(\mathbf{x}_u) dx_i = 0 \text{ for } i \in u \neq \emptyset,\ \mathbf{j}_u \in \mathbb{N}^{|u|}. \tag{5}$$

They produce two remarkable properties of random orthogonal polynomials: (1) each polynomial $P_{u,\mathbf{j}_u}(\mathbf{x}_u)$, where $\emptyset \neq u \subseteq \{1, \ldots, N\}$ and $\mathbf{j}_u \in \mathbb{N}^{|u|}$, has a zero mean; and (2) two distinct polynomials $P_{u,\mathbf{j}_u}(\mathbf{x}_u)$ and $P_{v,\mathbf{k}_v}(\mathbf{x}_v)$, where $\emptyset \neq u, v \subseteq \{1, \ldots, N\}$, $v \subset u$, $\mathbf{j}_u \in \mathbb{N}^{|u|}$, and $\mathbf{k}_v \in \mathbb{N}^{|v|}$, are orthogonal. They lead to the following second-moment properties of $\Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)$.

3.4.2. Second-moment properties

For $\emptyset \neq u, v \subseteq \{1, \ldots, N\}$, $\mathbf{j}_u \in \mathbb{N}^{|u|}$, and $\mathbf{k}_v \in \mathbb{N}^{|v|}$, the first- and second-order moments of standardized multivariate orthogonal polynomials, respectively, are

$$\mathbb{E}\left[\Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)\right] = 0 \tag{6}$$

and

$$\mathbb{E}\left[\Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)\,\Psi_{v,\mathbf{k}_v}(\mathbf{X}_v)\right] = \begin{cases} 0, & u \subset v \subset u, \forall\, \mathbf{j}_u, \mathbf{k}_v, \\ 0, & \forall\, u, v, |\mathbf{j}_u| \neq |\mathbf{k}_v|, \\ 1, & u = v, \mathbf{j}_u = \mathbf{k}_v, \\ \displaystyle\int_{\mathbb{A}^{u\cup v}} \Psi_{u,\mathbf{j}_u}(\mathbf{x}_u)\,\Psi_{v,\mathbf{k}_v}(\mathbf{x}_v) f_{\mathbf{X}_{u\cup v}}(\mathbf{x}_{u\cup v}) d\mathbf{x}_{u\cup v}, & \text{otherwise.} \end{cases} \tag{7}$$

Here, the two orthogonality conditions of (7) deserve attention. The condition in the first line stems from the weak annihilating conditions (5) obeyed by $P_{u,\mathbf{j}_u}(\mathbf{x}_u)$. The orthogonality holds for any nested subsets $u \subset v \subset u$, but for arbitrary $\mathbf{j}_u \in \mathbb{N}^{|u|}$, $\mathbf{k}_v \in \mathbb{N}^{|v|}$. The condition in the second line is rooted in the definition of orthogonal polynomials in $\mathbf{x}$, that is, in (3) for $u = \{1, \ldots, N\}$. The non-trivial expressions of (7) come from their definitions. No further reduction is possible for a general probability measure.

When $\mathbf{X} = (X_1, \ldots, X_N)^T$ comprises independent, but not necessarily identical, input random variables, the multivariate polynomials are usually built from the tensor product of univariate polynomials, and the second-moment properties simplify substantially. Denote by $f_{X_i}(x_i)$, $i = 1, \ldots, N$, the marginal density function of the ith random variable X_i and by $\Psi_{\{i\},j_i}(x_i)$ the j_ith-degree univariate orthonormal polynomial in x_i, which is obtained consistent with the probability measure $f_{X_i}(x_i)dx_i$. Then, for $\emptyset \neq u \subseteq \{1, \ldots, N\}$, $\mathbf{j}_u \in \mathbb{N}^{|u|}$,

$$\Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) = \prod_{i\in u} \Psi_{\{i\},j_i}(x_i) = \prod_{p=1}^{|u|} \Psi_{\{i_p\},j_{i_p}}(x_{i_p})$$

is a multivariate orthonormal polynomial in $\mathbf{x}_u = (x_{i_1}, \ldots, x_{i_{|u|}})$ of degree $|\mathbf{j}_u| = j_{i_1} + \cdots + j_{i_{|u|}}$. Consequently, for $\emptyset \neq u, v \subseteq \{1, \ldots, N\}$, $\mathbf{j}_u \in \mathbb{N}^{|u|}$, and $\mathbf{k}_v \in \mathbb{N}^{|v|}$, the first- and second-order moments of multivariate orthonormal polynomials, respectively, are

$$\mathbb{E}\left[\Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)\right] = 0 \tag{8}$$

and

$$\mathbb{E}\left[\Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)\,\Psi_{v,\mathbf{k}_v}(\mathbf{X}_v)\right] = \begin{cases} 1, & u = v,\ \mathbf{j}_u = \mathbf{k}_v, \\ 0, & \text{otherwise.} \end{cases} \tag{9}$$

The simplified results of (8) and (9), readily exploited by the existing PDD [11], are no longer valid for dependent variables, which are the focus of this paper.

3.5. A special class of orthogonal polynomials

Consider a family of probability measures, where the probability density function of $\mathbf{X}_u$, $\emptyset \neq u \subseteq \{1, \ldots, N\}$, has derivatives of all orders, that is, $f_{\mathbf{X}_u} \in C^\infty(\mathbb{A}^N)$, where $C^\infty(\mathbb{A}^N)$ represents the class of infinitely differentiable functions on $\mathbb{A}^N$. In such a case, there exists a special class of multivariate orthogonal polynomials in $\mathbf{x}_u$ that can be generated directly from the derivatives of the density function, leading to a Rodrigues type formula:

$$P_{u,\mathbf{j}_u}(\mathbf{x}_u) f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\alpha}_u) \propto \left(\frac{\partial}{\partial \mathbf{x}_u}\right)^{\mathbf{j}_u} f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\beta}_u(\boldsymbol{\alpha}_u,\mathbf{j}_u)),\ \emptyset \neq u \subseteq \{1, \ldots, N\},\ \mathbf{j}_u \in \mathbb{N}^{|u|}. \tag{10}$$

Here, $\boldsymbol{\alpha}_u$ is a vector of real-valued parameters describing $f_{\mathbf{X}_u}$; $\boldsymbol{\beta}_u$, depending on the choice of $f_{\mathbf{X}_u}$, is a function of $\boldsymbol{\alpha}_u$ and $\mathbf{j}_u$; $f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\alpha}_u) = f_{\mathbf{X}_u}(\mathbf{x}_u)$ is an additional symbol for the same density function but with the parameters explicitly shown as arguments; and $(\partial/\partial \mathbf{x}_u)^{\mathbf{j}_u} := \partial^{j_{i_1}+\cdots+j_{i_{|u|}}}/\partial x_{i_1}^{j_{i_1}} \cdots \partial x_{i_{|u|}}^{j_{i_{|u|}}}$.

Three commonly used probability density functions for which the formula (10) can be applied are (1) Gaussian density on the real space $\mathbb{R}^{|u|}$, (2) Gegenbauer or ultraspherical density on the unit ball $\mathbb{B}^{|u|} := \{\mathbf{x}_u \in \mathbb{R}^{|u|} : \|\mathbf{x}_u\| := (x_{i_1}^2 + \cdots + x_{i_{|u|}}^2)^{1/2} \leq 1\}$, and (3) Dirichlet density on the standard simplex $\mathbb{T}^{|u|} := \{\mathbf{x}_u \in \mathbb{R}^{|u|} : x_{i_1} \geq 0, \ldots, x_{i_{|u|}} \geq 0, |\mathbf{x}_u| := x_{i_1} + \cdots + x_{i_{|u|}} \leq 1\}$. The associated polynomials are referred to as multivariate Hermite, Gegenbauer, and Dirichlet polynomials, respectively. Explicit forms of these density functions and formulae are described as follows.

3.5.1. Gaussian density on $\mathbb{R}^{|u|}$ [20,25]

$$f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\alpha}_u) = (2\pi)^{-\frac{|u|}{2}}\left(\det \boldsymbol{\Sigma}_{\mathbf{X}_u}\right)^{-\frac{1}{2}} \exp\left[-\frac{1}{2}\mathbf{x}_u^T\boldsymbol{\Sigma}_{\mathbf{X}_u}^{-1}\mathbf{x}_u\right],\ \mathbf{x}_u \in \mathbb{R}^{|u|},$$

$$\Sigma_{\mathbf{X}_u} = \begin{bmatrix} \sigma_{i_1}^2 & \rho_{i_1i_2}\sigma_{i_1}\sigma_{i_2} & \cdots & \rho_{i_1i_{|u|}}\sigma_{i_1}\sigma_{i_{|u|}} \\ & \sigma_{i_2}^2 & \cdots & \rho_{i_2i_{|u|}}\sigma_{i_2}\sigma_{i_{|u|}} \\ & & \ddots & \vdots \\ \text{(sym.)} & & \cdots & \sigma_{i_{|u|}}^2 \end{bmatrix} \text{ (must be positive-definite)},$$

$$0 < \sigma_{i_p} < \infty,\ -1 < \rho_{i_pi_q} < +1,\ 1 \le p, q \le |u|,\ i_p, i_q \in u,$$

$$\boldsymbol{\alpha}_u = (\sigma_{i_1}, \ldots, \sigma_{i_{|u|}}; \rho_{i_1i_2}, \ldots, \rho_{i_{|u|-1}i_{|u|}}) \in \mathbb{R}^{\frac{|u|+|u|^2}{2}},\ \boldsymbol{\beta}_u = \boldsymbol{\alpha}_u,$$

$$P_{u,\mathbf{j}_u}(\mathbf{x}_u) f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\alpha}_u) \propto \left(\frac{\partial}{\partial \mathbf{x}_u}\right)^{\mathbf{j}_u} \exp\left[-\frac{1}{2}\mathbf{x}_u^T\boldsymbol{\Sigma}_{\mathbf{X}_u}^{-1}\mathbf{x}_u\right].$$

3.5.2. Gegenbauer density on $\mathbb{B}^{|u|}$ [19,20,22]

$$f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\alpha}_u) = \frac{\Gamma\left(\mu_u + \frac{|u|+1}{2}\right)}{\pi^{\frac{|u|}{2}}\Gamma\left(\mu_u + \frac{1}{2}\right)}\left(1 - \|\mathbf{x}_u\|^2\right)^{\mu_u - \frac{1}{2}},\ \|\mathbf{x}_u\|^2 := x_{i_1}^2 + \cdots + x_{i_{|u|}}^2,\ \mathbf{x}_u \in \mathbb{B}^{|u|},$$

$$\mu_u > -\frac{1}{2},\ \boldsymbol{\alpha}_u = (\mu_u) \in \mathbb{R},\ \boldsymbol{\beta}_u = (|\mathbf{j}_u| + \mu_u) \in \mathbb{R},$$

$$P_{u,\mathbf{j}_u}(\mathbf{x}_u) f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\alpha}_u) \propto \left(\frac{\partial}{\partial \mathbf{x}_u}\right)^{\mathbf{j}_u}\left(1 - \|\mathbf{x}_u\|^2\right)^{|\mathbf{j}_u| + \mu_u - \frac{1}{2}}.$$

3.5.3. Dirichlet density on $\mathbb{T}^{|u|}$ [19,20,22]

$$f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\alpha}_u) = \frac{\Gamma\left(\sum_{p=1}^{|u|+1}\kappa_{u,i_p} + \frac{|u|+1}{2}\right)}{\prod_{p=1}^{|u|+1}\Gamma\left(\kappa_{u,i_p} + \frac{1}{2}\right)}\left(\prod_{p=1}^{|u|} x_{i_p}^{\kappa_{u,i_p} - \frac{1}{2}}\right)\left(1 - |\mathbf{x}_u|\right)^{\kappa_{u,i_{|u|+1}} - \frac{1}{2}},$$

$$|\mathbf{x}_u| := x_{i_1} + \cdots + x_{i_{|u|}},\ \mathbf{x}_u \in \mathbb{T}^{|u|},$$

$$\kappa_{u,i_p} > -\frac{1}{2},\ p = 1, \ldots, |u|+1,\ \boldsymbol{\alpha}_u = (\kappa_{u,i_1}, \ldots, \kappa_{u,i_{|u|+1}}) \in \mathbb{R}^{|u|+1},$$

$$\boldsymbol{\beta}_u = (\kappa_{u,i_1} + j_{i_1}, \ldots, \kappa_{u,i_{|u|+1}} + j_{i_{|u|+1}}) \in \mathbb{R}^{|u|+1},$$

$$P_{u,\mathbf{j}_u}(\mathbf{x}_u) f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\alpha}_u) \propto \left(\frac{\partial}{\partial \mathbf{x}_u}\right)^{\mathbf{j}_u}\left[\left(\prod_{p=1}^{|u|} x_{i_p}^{\kappa_{u,i_p} - \frac{1}{2} + j_{i_p}}\right)\left(1 - |\mathbf{x}_u|\right)^{\kappa_{u,i_{|u|+1}} - \frac{1}{2} + |\mathbf{j}_u|}\right].$$

The Gaussian distribution is well known and often used in natural, applied, and social sciences. The Gegenbauer distribution or polynomials find their applications in engineering or mathematics, for instance, in potential theory and harmonic analysis. The Dirichlet distribution is frequently employed in Bayesian statistics.

Note that the specific forms of (10) written for the Gaussian and Gegenbauer distributions mandate that the input random vectors $\mathbf{X}$ have *zero* means. Conversely, if the mean $\mathbb{E}[\mathbf{X}]$ is not *zero*, then the same formula can be used working with the shifted input random vector $\mathbf{X} - \mathbb{E}[\mathbf{X}]$. In other words, (10), if it exists, is also applicable for random input with non-zero means. All three distributions will be revisited in Section 5 where numerical examples are presented.

Formula (10) is also useful in proving that the resultant orthogonal polynomials satisfy (5). This is demonstrated in Appendix A when the probability density function has a compact support, such as the Gegenbauer and Dirichlet distributions, or has an unbounded support where the density function converges to *zero* faster than the rate at which polynomials become unbounded at the boundary, such as the Gaussian distribution. It is important, however, to clarify that although (5) and (A.1) state the same result, the former is more general than the latter, and is applicable to any measure-consistent orthogonal polynomials. In either case, the result is valid as long as $\mathbf{j}_u \in \mathbb{N}^{|u|}$, that is, the power j_{i_p} of the i_pth variable, where $i_p \in u \subseteq \{1,\ldots,N\}$, $p = 1,\ldots,|u|$, and $|u| > 0$, takes on positive integer values.

4. Generalized polynomial dimensional decomposition

Let $y(\mathbf{X}) := y(X_1,\ldots,X_N)$ be a real-valued, square-integrable output random variable defined on the same probability space $(\Omega,\mathcal{F},\mathbb{P})$. The vector space $L^2(\Omega,\mathcal{F},\mathbb{P})$ is a Hilbert space such that

$$\mathbb{E}\left[y^2(\mathbf{X})\right] := \int_{\Omega} y^2(\mathbf{X}(\omega))d\mathbb{P}(\omega) = \int_{\mathbb{A}^N} y^2(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x})d\mathbf{x} < \infty.$$

It is elementary to show that $y(\mathbf{X}(\omega)) \in L^2(\Omega,\mathcal{F},\mathbb{P})$ if and only if $y(\mathbf{x}) \in L^2(\mathbb{A}^N,\mathcal{B}^N, f_{\mathbf{X}}d\mathbf{x})$.

4.1. Generalized ADD

Under Assumption (4), a square-integrable function $y(\mathbf{X}) \in L^2(\Omega,\mathcal{F},\mathbb{P})$ of input variables $\mathbf{X}$ admits a unique, finite, hierarchical expansion [26]

$$y(\mathbf{X}) = y_\emptyset + \sum_{\emptyset\neq u\subseteq\{1,\ldots,N\}} y_u(\mathbf{X}_u), \tag{11a}$$

$$y_\emptyset = \int_{\mathbb{A}^N} y(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x})d\mathbf{x}, \tag{11b}$$

$$y_u(\mathbf{X}_u) = \int_{\mathbb{A}^{-u}} y(\mathbf{X}_u,\mathbf{x}_{-u}) f_{\mathbf{X}_{-u}}(\mathbf{x}_{-u})d\mathbf{x}_{-u} - \sum_{v\subset u} y_v(\mathbf{X}_v) - \sum_{\substack{\emptyset\neq v\subseteq\{1,\ldots,N\}\\ v\cap u\neq\emptyset, v\not\subseteq u}} \int_{\mathbb{A}^{v\cap -u}} y_v(\mathbf{X}_{v\cap u},\mathbf{x}_{v\cap -u}) f_{\mathbf{X}_{v\cap -u}}(\mathbf{x}_{v\cap -u})d\mathbf{x}_{v\cap -u}, \tag{11c}$$

in terms of its input variables with increasing dimensions, where $u \subseteq \{1,\ldots,N\}$ is a subset with the complementary set $-u = \{1,\ldots,N\}\setminus u$ and y_u is a $|u|$-variate component function describing a constant or an $|u|$-variate interaction of $\mathbf{X}_u = (X_{i_1},\ldots,X_{i_{|u|}})$ on y when $|u| = 0$ or $|u| > 0$. This expansion is known as the generalized ADD [26]. Although it was originally derived using $\mathbb{A}^N = \mathbb{R}^N$ [26], the extension for the case of $\mathbb{A}^N \subseteq \mathbb{R}^N$ is trivial. Here, $(\mathbf{X}_u,\mathbf{x}_{-u})$ denotes an N-dimensional vector whose ith component is X_i if $i \in u$ and x_i if $i \notin u$. Similar to the classical ADD, the summation in (11a) comprises $2^N - 1$ terms with each term depending on a group of variables indexed by a particular subset of $\{1,\ldots,N\}$. When $u = \emptyset$, both sums in (11c) vanish, resulting in the expression of the constant function $y_\emptyset$ in (11b). When $u = \{1,\ldots,N\}$, the integration in the first line of (11c) is on the empty set and the sum in the second line of (11c) vanishes, reproducing (11a) and hence finding the last function $y_{\{1,\ldots,N\}}$. Indeed, all component functions of y can be obtained by interpreting literally (11c).

The generalized ADD described by (11a)–(11c) has two notable properties [26,27]: (1) the component functions y_u, where $\emptyset \neq u \subseteq \{1,\ldots,N\}$, have zero means, that is,

$$\mathbb{E}\left[y_u(\mathbf{X}_u)\right] = 0; \tag{12}$$

and (2) two distinct component functions $y_{u,G}$ and $y_{v,G}$, where $\emptyset \neq u \subseteq \{1,\ldots,N\}$, $\emptyset \neq v \subseteq \{1,\ldots,N\}$, and $v \subset u$, are orthogonal, that is, they satisfy the property

$$\mathbb{E}\left[y_u(\mathbf{X}_u)y_v(\mathbf{X}_v)\right] = 0. \tag{13}$$

These properties originate from enforcing similar weak annihilating conditions on the generalized ADD component functions y_u [27]. Readers interested in further details are directed to a prior work of the author [26].

4.2. Generalized PDD

The GPDD of a random variable $y(\mathbf{X}) \in L^2(\Omega, \mathcal{F}, \mathbb{P})$ is simply the expansion of $y(\mathbf{X})$ with respect to a complete, hierarchically ordered, orthogonal polynomial basis of $L^2(\Omega, \mathcal{F}, \mathbb{P})$.

Theorem 1. *Let $\mathbf{X} := (X_1, \ldots, X_N)^T$ be a vector of $N \in \mathbb{N}$ input random variables fulfilling Assumptions (1)-(4). For $\emptyset \neq u \subseteq \{1, \ldots, N\}$ and $\mathbf{X}_u := (X_{i_1}, \ldots, X_{i_{|u|}})^T : (\Omega^u, \mathcal{F}^u) \to (\mathbb{A}^u, \mathcal{B}^u)$, denote by $\{\Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) : \mathbf{j}_u \in \mathbb{N}^{|u|}\}$ the set of standardized multivariate orthogonal polynomials consistent with the probability measure $f_{\mathbf{X}_u}(\mathbf{x}_u)d\mathbf{x}_u$. Then for any random variable $y(\mathbf{X}) \in L^2(\Omega, \mathcal{F}, \mathbb{P})$ there exists a Fourier-like series in multivariate orthogonal polynomials in $\mathbf{X}$, referred to as the GPDD of*

$$y(\mathbf{X}) \sim y_\emptyset + \sum_{\emptyset \neq u \subseteq \{1,\ldots,N\}} \sum_{\mathbf{j}_u \in \mathbb{N}^{|u|}} C_{u,\mathbf{j}_u} \Psi_{u,\mathbf{j}_u}(\mathbf{X}_u), \tag{14}$$

where the zero-*variate, expansion coefficient $y_\emptyset \in \mathbb{R}$ is defined by*

$$y_\emptyset := \mathbb{E}[y(\mathbf{X})] := \int_{\mathbb{A}^N} y(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \tag{15}$$

and the $|u|$-variate, $|\mathbf{j}_u|$th-order expansion coefficients $C_{u,\mathbf{j}_u} \in \mathbb{R}$ satisfy the infinite-dimensional linear system

$$\sum_{\emptyset \neq v \subseteq \{1,\ldots,N\}} \sum_{\mathbf{k}_v \in \mathbb{N}^{|v|}} C_{v,\mathbf{k}_v} J_{u,\mathbf{j}_u;v,\mathbf{k}_v} = I_{u,\mathbf{j}_u}, \ \emptyset \neq u \subseteq \{1,\ldots,N\}, \ \mathbf{j}_u \in \mathbb{N}^{|u|}, \tag{16}$$

with the integrals

$$I_{u,\mathbf{j}_u} := \mathbb{E}\left[y(\mathbf{X}) \Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)\right] := \int_{\mathbb{A}^N} y(\mathbf{x}) \Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x}, \tag{17a}$$

$$J_{u,\mathbf{j}_u;v,\mathbf{k}_v} := \mathbb{E}\left[\Psi_{u,\mathbf{j}_u}(\mathbf{X}_u) \Psi_{v,\mathbf{k}_v}(\mathbf{X}_v)\right] := \int_{\mathbb{A}^N} \Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) \Psi_{v,\mathbf{k}_v}(\mathbf{x}_v) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x}. \tag{17b}$$

Furthermore, the GPDD of $y(\mathbf{X}) \in L^2(\Omega, \mathcal{F}, \mathbb{P})$ converges to $y(\mathbf{X})$ in mean-square, in probability, and in distribution. Here, the symbol $\sim$ in (14) represents equality in a weaker sense, such as equality in mean-square, but not necessarily pointwise nor almost everywhere.

Proof. For a complete proof, see the companion paper [18]. Here, an alternative proof, not available elsewhere, deriving only the equations involving the expansion coefficients is presented.

Applying the expectation operator on (14) and using the *zero*-mean property of $\Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)$ from (6) results in (15). To obtain (16), replace $y(\mathbf{X})$ in (17a) with the full GPDD, that is, (14), producing

$$\begin{aligned}
I_{u,\mathbf{j}_u} &= \int_{\mathbb{A}^N} \left[y_\emptyset + \sum_{\emptyset \neq v \subseteq \{1,\ldots,N\}} \sum_{\mathbf{k}_v \in \mathbb{N}^{|v|}} C_{v,\mathbf{k}_v} \Psi_{v,\mathbf{k}_v}(\mathbf{X}_v) \right] \Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \\
&= \int_{\mathbb{A}^N} y_\emptyset \Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} + \int_{\mathbb{A}^N} \sum_{\emptyset \neq v \subseteq \{1,\ldots,N\}} \sum_{\mathbf{k}_v \in \mathbb{N}^{|v|}} C_{v,\mathbf{k}_v} \Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) \Psi_{v,\mathbf{k}_v}(\mathbf{X}_v) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \\
&= \int_{\mathbb{A}^N} \sum_{\emptyset \neq v \subseteq \{1,\ldots,N\}} \sum_{\mathbf{k}_v \in \mathbb{N}^{|v|}} C_{v,\mathbf{k}_v} \Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) \Psi_{v,\mathbf{k}_v}(\mathbf{X}_v) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \\
&= \sum_{\emptyset \neq v \subseteq \{1,\ldots,N\}} \sum_{\mathbf{k}_v \in \mathbb{N}^{|v|}} C_{v,\mathbf{k}_v} \int_{\mathbb{A}^N} \Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) \Psi_{v,\mathbf{k}_v}(\mathbf{X}_v) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x}.
\end{aligned}$$

Here, the third line is attained by applying (6) to the second line, annihilating the first integral. The last line is obtained by switching the orders of integral and summation operators, which is permissible as the infinite series of GPDD is a convergent sum [18]. Finally, invoking the definition of $J_{u,\mathbf{j}_u;v,\mathbf{k}_v}$ in (17b) results in (16). □

The infinite system (16) can be reduced further as many of the integral coefficients, that is, $J_{u,\mathbf{j}_u;v,\mathbf{k}_v}$, vanish conforming to (7). Indeed, as $J_{u,\mathbf{j}_u;v,\mathbf{k}_v} = 0$ for $|\mathbf{j}_u| \neq |\mathbf{k}_v|$, (16) is actually an infinite system of uncoupled finite-dimensional linear systems. Moreover, the system matrix of each finite-dimensional system is sparse, because

$J_{u,\mathbf{j}_u;v,\mathbf{k}_v} = 0$ for $u \subset v \subset u$. Some of these issues will be revisited in a forthcoming section devoted to the expansion coefficients of a truncated GPDD.

It should be emphasized that the function y must be square-integrable for the mean-square and other convergences to hold. However, the rate of convergence depends on the smoothness of the function. The smoother the function, the faster the convergence. If the function is a polynomial, then its GPDD exactly reproduces the function. These results can be easily proved using classical approximation theory.

4.2.1. Relationship with the generalized ADD

The GPDD proposed is surely connected to the generalized ADD. For instance, comparing (14) and (11a) reveals

$$y_u(\mathbf{X}_u) \sim \sum_{\mathbf{j}_u \in \mathbb{N}^{|u|}} C_{u,\mathbf{j}_u} \Psi_{u,\mathbf{j}_u}(\mathbf{X}_u), \tag{18}$$

indicating a clear affiliation between GPDD and the generalized ADD. Indeed, the former can be conceived as a polynomial adaptation of the latter. Here, $C_{u,\mathbf{j}_u} \Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)$ in (14) or (18) represents a $|u|$-variate, $|\mathbf{j}_u|$th-order GPDD component function of $y(\mathbf{X})$, describing the $|\mathbf{j}_u|$th-order polynomial approximation of the $|u|$-variate component function $y_u(\mathbf{X}_u)$ of the generalized ADD.

Moreover, given the statistical properties of multivariate orthogonal polynomials in (6) and (7), it is easy to verify that the second-moment properties of $y_u(\mathbf{X}_u)$, that is, (12) and (13), are naturally satisfied when $y_u(\mathbf{X}_u)$ is expanded as in (18). Therefore, GPDD inherits all desirable traits of the generalized ADD — an important prerequisite for any refinement of the latter.

4.2.2. A special case of independent variables

When $\mathbf{X} = (X_1, \ldots, X_N)^T$ comprises independent, but not necessarily identical, input random variables, denote by $f_{X_i}(x_i)$, $i = 1, \ldots, N$, the marginal density function of the ith random variable X_i and by $\Psi_{\{i\},j_i}(x_i)$ the j_ith-degree univariate orthonormal polynomial in x_i, which is obtained consistent with the probability measure $f_{X_i}(x_i)dx_i$. Then one can write: $f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^{N} f_{X_i}(x_i)$ and $\Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) = \prod_{p=1}^{|u|} \Psi_{\{i_p\},j_{i_p}}(x_{i_p})$. In addition, from (9), the integral $J_{u,\mathbf{j}_u;v,\mathbf{k}_v} = 1$ when $u = v$ and $\mathbf{j}_u = \mathbf{k}_v$, and *zero* otherwise. As a result, the proposed GPDD reduces to the existing PDD, yielding

$$y(\mathbf{X}) \sim y_\emptyset + \sum_{\emptyset \neq u \subseteq \{1,\ldots,N\}} \sum_{\mathbf{j}_u \in \mathbb{N}^{|u|}} C_{u,\mathbf{j}_u} \prod_{p=1}^{|u|} \Psi_{\{i_p\},j_{i_p}}(X_{i_p})$$

with the expansion coefficients

$$y_\emptyset = \mathbb{E}\left[y(\mathbf{X})\right] = \int_{\mathbb{A}^N} y(\mathbf{x}) \prod_{i=1}^{N} f_{X_i}(x_i)dx_i$$

and

$$C_{u,\mathbf{j}_u} = \mathbb{E}\left[y(\mathbf{X}) \prod_{p=1}^{|u|} \Psi_{\{i_p\},j_{i_p}}(X_{i_p}) \right] := \int_{\mathbb{A}^N} y(\mathbf{x}) \prod_{p=1}^{|u|} \Psi_{\{i_p\},j_{i_p}}(x_{i_p}) \prod_{i=1}^{N} f_{X_i}(x_i)dx_i .$$

4.3. Truncation

The full GPDD contains an infinite number of orthogonal polynomials or coefficients. In practice, the number must be finite, meaning that GPDD must be truncated. However, there are multiple ways to perform the truncation. A straightforward approach adopted in this work entails (1) keeping all polynomials in at most $0 \leq S \leq N$ variables, thereby retaining the degrees of interaction among input variables less than or equal to S, and (2) preserving polynomial expansion orders (total) less than or equal to $S \leq m < \infty$. The result is an S-variate, mth-order GPDD

approximation[3]

$$y_{S,m}(\mathbf{X}) = y_{\emptyset} + \sum_{\substack{\emptyset \neq u \subseteq \{1,\ldots,N\} \\ 1 \le |u| \le S}} \sum_{\substack{\mathbf{j}_u \in \mathbb{N}^{|u|} \\ |u| \le |\mathbf{j}_u| \le m}} C_{u,\mathbf{j}_u} \Psi_{u,\mathbf{j}_u}(\mathbf{X}_u) \tag{19}$$

of $y(\mathbf{X})$. It is important to clarify a few things about the truncated GPDD proposed. First, the truncation with respect to the expansion order in (19) is related to the total degree index set

$$\left\{ \mathbf{j}_u \in \mathbb{N}^{|u|} : \sum_{p=1}^{|u|} j_{i_p} \le m \right\}.$$

Other kinds of truncation involve the tensor product and hyperbolic cross index sets, but they were not considered in this work. Second, for the total degree index set, the minimum value of m must be S. If $m < S$, then for $m < |u| \le S$ there are no $|u|$-variate, mth-order polynomials in (19). Third, the right side of (19) contains sums of at most S-dimensional orthogonal polynomials, representing at most S-variate GPDD component functions of y. Therefore, the term "S-variate" used for the GPDD approximation should be interpreted in the context of including at most S-degree interaction of input variables, even though $y_{S,m}$ is strictly an N-variate function. Fourth, when $S = 0$, $y_{0,m} = y_{\emptyset}$ for any m as the outer sums of (19) vanish. Finally, when $S \to N$ and $m \to \infty$, $y_{S,m}$ converges to y in the mean-square sense, generating a hierarchical and convergent sequence of GPDD approximations.

The motivation behind generalized ADD- and GPDD-derived approximations is the following. In a practical setting, the function $y(\mathbf{X})$, fortunately, has an effective dimension much lower than N, meaning that the right side of (11a) can be effectively approximated by a sum of lower-dimensional component functions y_u, $|u| \ll N$, but still maintaining all random variables $\mathbf{X}$ of a high-dimensional UQ problem. For instance, an S-variate, mth-order GPDD approximation $y_{S,m}(\mathbf{X})$ is generated, where $0 \le S \le N$ and $S \le m < \infty$ define the largest degree of interactions among input variables and the largest order of orthogonal polynomials retained in a concomitant truncation. The approximation is grounded on a fundamental conjecture known to be true in many real-world problems: given a high-dimensional function y, its $|u|$-variate, $|\mathbf{j}_u|$th-order GPDD component function $C_{u,\mathbf{j}_u} \Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)$ decays rapidly with respect to $|u|$ and $|\mathbf{j}_u|$, leading to an accurate low-variate, low-order approximation of y.

4.4. Computational effort

Due to identical hierarchical structures of function decompositions, the GPDD method has the same computational complexity as the existing PDD method. To expound on the scalability of GPDD with respect to the problem size or the number of random variables N, consider two special cases of approximations: the one representing the univariate ($S = 1$), mth-order GPDD approximation

$$y_{1,m}(\mathbf{X}) = y_{\emptyset} + \sum_{i=1}^{N} \sum_{j_i=1}^{m} C_{\{i\},j_i} \Psi_{\{i\},j_i}(X_i) \tag{20}$$

and the other describing the bivariate ($S = 2$), mth-order GPDD approximation

$$\begin{aligned} y_{2,m}(\mathbf{X}) \;=\; & y_{\emptyset} + \sum_{i=1}^{N} \sum_{j_i=1}^{m} C_{\{i\},j_i} \Psi_{\{i\},j_i}(X_i) \\ & + \sum_{i_1=1}^{N-1} \sum_{i_2=i_1+1}^{N} \sum_{\substack{(j_{i_1},j_{i_2}) \in \mathbb{N}^2 \\ 2 \le j_{i_1}+j_{i_2} \le m}} C_{\{i_1,i_2\},(j_{i_1},j_{i_2})} \Psi_{\{i_1,i_2\},(j_{i_1},j_{i_2})}(X_{i_1}, X_{i_2}). \end{aligned} \tag{21}$$

Analogs of these two approximations, obtained from the existing PDD method, are frequently used for solving large-scale UQ problems [28–31]. In either case, the computational effort is proportional to the respective number of expansion coefficients involved. Therefore, the computational effort of a GPDD or PDD approximation can be judged by the number of coefficients. For instance, in (20) and (21), there are respectively

$$1 + Nm$$

[3] The nouns *degree* and *order* associated with GPDD or orthogonal polynomials are used synonymously in the paper.

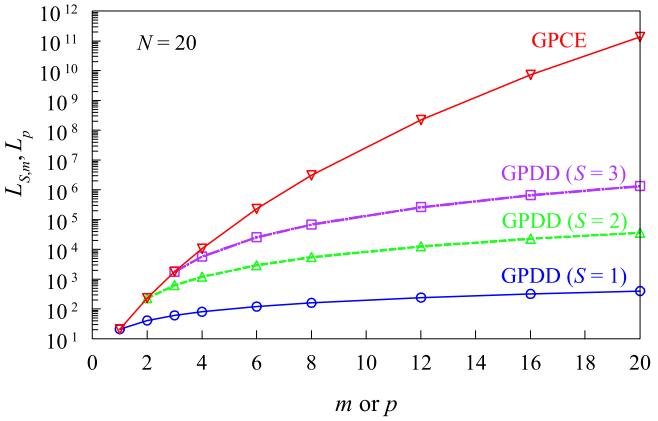


Fig. 1. Growth of expansion coefficients in the GPDD and GPCE approximations.

and

$$1 + Nm + \frac{N(N-1)}{2}\frac{m(m-1)}{2}$$

numbers of coefficients. Hence, given a fixed value of m, the computational effort with respect to N grows linearly for univariate approximation and quadratically for bivariate approximation. For example, when $N = 20$ and $m = 2$, the univariate, second-order GPDD approximation and the bivariate, second-order GPDD approximation require 41 and 231 expansion coefficients, respectively. Following similar considerations, the number of expansion coefficients for a general S-variate, mth-order GPDD approximation in (19) is

$$L_{S,m} = 1 + \sum_{s=1}^{S} \binom{N}{s}\binom{m}{s}, \tag{22}$$

including $y_\emptyset$. Therefore, the computational effort by an S-variate, mth-order GPDD approximation scales S-degree-polynomially with respect to N. The same formula (22) applies for determining the expansion coefficients of the respective PDD approximation valid for independent random variables [11]. Indeed, the computational complexity of a truncated GPDD or PDD is polynomial, as opposed to exponential, thereby alleviating the curse of dimensionality to a substantial extent.

Finally, to understand better the computational effort of GPDD, contrasting it with the recently developed generalized polynomial chaos expansion (GPCE) [32], also valid for dependent variables, should be interesting. When truncated according to the total degree index set, the pth-order GPCE approximation of $y(\mathbf{X})$ comprises $L_p = (N + p)!/(N!p!)$ number of expansion coefficients. For a problem size of $N = 20$, Fig. 1 presents four plots explaining how the required numbers of expansion coefficients – $L_{S,m}$ for GPDD and L_p for GPCE – rise with respect to the order m or p. For GPDD, three plots for distinct values of $S = 1$, $S = 2$, and $S = 3$, representing univariate, bivariate, and trivariate approximations, respectively, are displayed. According to Fig. 1, the growth of the number of expansion coefficients in GPCE is much steeper than that in GPDD. The number of expansion coefficients escalates significantly when the polynomial expansion order is large. This is primarily because a GPCE approximation is wholly prescribed by a single truncation parameter p, which determines the largest polynomial expansion order preserved, but not the degree of interaction freely. In contrast, there are two different truncation parameters S and m in a GPDD approximation, supporting a greater adaptability in retaining the largest degree of interaction and largest polynomial expansion order. Consequently, the GPDD approximation can be decidedly more computationally efficient than the GPCE approximation.

4.5. Expansion coefficients

According to (19), determining the expansion coefficients of the S-variate, mth-order GPDD approximation requires solving an $(L_{S,m} \times L_{S,m})$ system of linear equations. However, as $J_{u,\mathbf{j}_u;v,\mathbf{k}_v}$ vanishes whenever $|\mathbf{j}_u| \neq |\mathbf{k}_v|$,

Table 1
A degree-wise arrangement for the expansion coefficients of $y_{3,4}$, $N = 3$.

$l = 1$	$l = 2$	$l = 3$	$l = 4$
$C_{\{1\},(1)}$	$C_{\{1\},(2)}$	$C_{\{1\},(3)}$	$C_{\{1\},(4)}$
$C_{\{2\},(1)}$	$C_{\{2\},(2)}$	$C_{\{2\},(3)}$	$C_{\{2\},(4)}$
$C_{\{3\},(1)}$	$C_{\{3\},(2)}$	$C_{\{3\},(3)}$	$C_{\{3\},(4)}$
	$C_{\{1,2\},(1,1)}$	$C_{\{1,2\},(2,1)}$	$C_{\{1,2\},(3,1)}$
	$C_{\{1,3\},(1,1)}$	$C_{\{1,2\},(1,2)}$	$C_{\{1,2\},(2,2)}$
	$C_{\{2,3\},(1,1)}$	$C_{\{1,3\},(2,1)}$	$C_{\{1,2\},(1,3)}$
		$C_{\{1,3\},(1,2)}$	$C_{\{1,3\},(3,1)}$
		$C_{\{2,3\},(2,1)}$	$C_{\{1,3\},(2,2)}$
		$C_{\{2,3\},(1,2)}$	$C_{\{1,3\},(1,3)}$
		$C_{\{1,2,3\},(1,1,1)}$	$C_{\{2,3\},(3,1)}$
			$C_{\{2,3\},(2,2)}$
			$C_{\{2,3\},(1,3)}$
			$C_{\{1,2,3\},(2,1,1)}$
			$C_{\{1,2,3\},(1,2,1)}$
			$C_{\{1,2,3\},(1,1,2)}$

the coefficients interact with each other only for a specific degree. Therefore, the coefficients for each degree can be determined independently.

Given $1 \le S \le N$ and $S \le m < \infty$, let $1 \le l \le m$ be an integer. Rearranging the expansion coefficients according to the degree l, the same S-variate, mth-order GPDD approximation can be written as

$$y_{S,m}(\mathbf{X}) = y_{\emptyset} + \sum_{l=1}^{m} \sum_{\substack{\emptyset \neq u \subseteq \{1,\ldots,N\} \\ 1 \le |u| \le \min(S,l)}} \sum_{\substack{\mathbf{j}_u \in \mathbb{N}^{|u|} \\ |\mathbf{j}_u| = l}} C_{u,\mathbf{j}_u} \Psi_{u,\mathbf{j}_u}(\mathbf{X}_u). \tag{23}$$

For each l, there are

$$Q_{S,l} = \sum_{s=1}^{\min(S,l)} \binom{N}{s} \binom{l-1}{s-1} \tag{24}$$

number of lth-degree orthogonal polynomials $\Psi_{u,\mathbf{j}_u}(\mathbf{x}_u)$ and corresponding expansion coefficients $C_{u,\mathbf{j}_u}$, where $1 \le |u| \le \min(S,l)$ and $|\mathbf{j}_u| = l$. To determine all such lth-degree interacting coefficients, only a $(Q_{S,l} \times Q_{S,l})$ linear system

$$\sum_{\substack{\emptyset \neq v \subseteq \{1,\ldots,N\} \\ 1 \le |v| \le \min(S,l)}} \sum_{\substack{\mathbf{k}_v \in \mathbb{N}^{|v|} \\ |\mathbf{k}_v| = |\mathbf{j}_u|}} C_{v,\mathbf{k}_v} J_{u,\mathbf{j}_u;v,\mathbf{k}_v} = I_{u,\mathbf{j}_u}, \ 1 \le |u| \le \min(S,l), \ |\mathbf{j}_u| = l, \tag{25}$$

has to be solved. The system matrix is a Gram matrix entailing moments of linearly independent orthogonal polynomials and is, therefore, positive-definite. As the matrix is positive-definite, it is invertible, meaning that a unique solution exists. When (25) is solved for $l = 1, \ldots, m$, then all $L_{S,m}$ expansion coefficients of (23) for degree at most m have been determined. Obviously,

$$L_{S,m} = \sum_{l=1}^{m} Q_{S,l}.$$

For illustration, consider a problem comprising three ($N = 3$) dependent random variables, where a trivariate ($S = 3$), fourth-order ($m = 4$) GPDD approximation is desired. Therefore, the degree of polynomials l runs from 1 to 4. For $l = 1, 2, 3$, and 4, Table 1 itemizes the expansion coefficients $C_{u,\mathbf{j}_u}$ from the condition: $1 \le |u| \le \min(S,l)$ and $|\mathbf{j}_u| = l$. The numbers of expansion coefficients listed in Table 1 agree with (24), for instance, $Q_{3,1} = 3$, $Q_{3,2} = 6$, $Q_{3,3} = 10$, and $Q_{3,4} = 15$. Therefore, to find all expansion coefficients of the aforementioned GPDD approximation, one can solve each group of the coefficients independently. It is easy to verify that the total number of coefficients, which is $3 + 6 + 10 + 15 = 34$, matches the value of $L_{3,4}$ from (22).

4.6. Output statistics and other probabilistic characteristics

The S-variate, mth-order PDD approximation $y_{S,m}(\mathbf{X})$ can be deemed as a surrogate of $y(\mathbf{X})$. Therefore, relevant probabilistic characteristics of $y(\mathbf{X})$, including its first two moments and probability density function, if it exists, can be assessed from the statistical properties of $y_{S,m}(\mathbf{X})$.

Proposition 2. *The truncated GPDD and GPDD have identical means*

$$\mathbb{E}\left[y_{S,m}(\mathbf{X})\right] = \mathbb{E}\left[y(\mathbf{X})\right] = y_{\emptyset} \tag{26}$$

that are exact, whereas their variances are

$$\mathrm{var}\left[y_{S,m}(\mathbf{X})\right] = \sum_{\substack{\emptyset \neq u,v \subseteq \{1,\ldots,N\} \\ 1 \le |u| \le S \\ 1 \le |v| \le S}} \sum_{\substack{\mathbf{j}_u \in \mathbb{N}^{|u|}, \mathbf{k}_v \in \mathbb{N}^{|v|} \\ |u| \le |\mathbf{j}_u| \le m \\ |v| \le |\mathbf{k}_v| \le m}} C_{u,\mathbf{j}_u} C_{v,\mathbf{k}_v} J_{u,\mathbf{j}_u;v,\mathbf{k}_v} \tag{27}$$

and

$$\mathrm{var}\left[y(\mathbf{X})\right] = \sum_{\emptyset \neq u,v \subseteq \{1,\ldots,N\}} \sum_{\mathbf{j}_u \in \mathbb{N}^{|u|}, \mathbf{k}_v \in \mathbb{N}^{|v|}} C_{u,\mathbf{j}_u} C_{v,\mathbf{k}_v} J_{u,\mathbf{j}_u;v,\mathbf{k}_v} \tag{28}$$

respectively. Moreover, the variance of the truncated GPDD converges to the variance of GPDD when $S \to N$ and $m \to \infty$.

Proof. Applying the expectation operator on $y_{S,m}(\mathbf{X})$ and $y(\mathbf{X})$ in (14) and (19) and imposing the second-moment properties of orthogonal polynomials in (6) and (7), their means are the same as $y_{\emptyset}$, the exact mean as per (26), and are independent of S and m. Therefore, GPDD truncated for any values of $0 \le S \le N$ and $S \le m < \infty$ yields the exact mean. Nonetheless, $\mathbb{E}[y_{S,m}(\mathbf{X})]$ will be referred to as the S-variate, mth-order GPDD approximation of the mean of $y(\mathbf{X})$.

Applying the expectation operator again, this time on $[y_{S,m}(\mathbf{X}) - y_{\emptyset}]^2$, produces

$$\begin{aligned}
\mathrm{var}\left[y_{S,m}(\mathbf{X})\right] &:= \mathbb{E}\left[y_{S,m}(\mathbf{X}) - y_{\emptyset}\right]^2 \\
&= \mathbb{E}\left[\sum_{\substack{\emptyset \neq u \subseteq \{1,\ldots,N\} \\ 1 \le |u| \le S}} \sum_{\substack{\mathbf{j}_u \in \mathbb{N}^{|u|} \\ |u| \le |\mathbf{j}_u| \le m}} C_{u,\mathbf{j}_u} \Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)\right]^2 \\
&= \mathbb{E}\left[\sum_{\substack{\emptyset \neq u,v \subseteq \{1,\ldots,N\} \\ 1 \le |u|,|v| \le S}} \sum_{\substack{\mathbf{j}_u \in \mathbb{N}^{|u|}, \mathbf{k}_v \in \mathbb{N}^{|v|} \\ |u| \le |\mathbf{j}_u| \le m \\ |v| \le |\mathbf{k}_v| \le m}} C_{u,\mathbf{j}_u} C_{v,\mathbf{k}_v} \Psi_{u,\mathbf{j}_u}(\mathbf{X}_u) \Psi_{v,\mathbf{k}_v}(\mathbf{X}_v)\right] \\
&= \sum_{\substack{\emptyset \neq u,v \subseteq \{1,\ldots,N\} \\ 1 \le |u|,|v| \le S}} \sum_{\substack{\mathbf{j}_u \in \mathbb{N}^{|u|}, \mathbf{k}_v \in \mathbb{N}^{|v|} \\ |u| \le |\mathbf{j}_u| \le m \\ |v| \le |\mathbf{k}_v| \le m}} C_{u,\mathbf{j}_u} C_{v,\mathbf{k}_v} J_{u,\mathbf{j}_u;v,\mathbf{k}_v}.
\end{aligned}$$

Here, the second line is obtained by employing (19); the third line is derived by expanding the square; and the last line is attained by interchanging the expectation and summation operators, followed by using the definition of the integral $J_{u,\mathbf{j}_u;v,\mathbf{k}_v}$ in (17b). Again, $\mathrm{var}[y_{S,m}(\mathbf{X})]$ will be referred to as the S-variate, mth-order GPDD approximation of the variance of $y(\mathbf{X})$. The derivation of (28) is similar. Clearly, $\mathrm{var}[y_{S,m}(\mathbf{X})]$ approaches $\mathrm{var}[y(\mathbf{X})]$, the exact variance of $y(\mathbf{X})$, as $S \to N$ and $m \to \infty$. □

When the input variables follow independent, but not necessarily identical, distributions, GPDD rolls back to the existing PDD, as alluded to in Section 4.2.2 already. In such a case, the means of the truncated PDD and PDD are also equal to $y_{\emptyset}$, but the expressions of respective variances simplify to

$$\mathrm{var}\left[y_{S,m}(\mathbf{X})\right] = \sum_{\substack{\emptyset \neq u \subseteq \{1,\ldots,N\} \\ 1 \le |u| \le S}} \sum_{\substack{\mathbf{j}_u \in \mathbb{N}^{|u|} \\ |u| \le |\mathbf{j}_u| \le m}} C_{u,\mathbf{j}_u}^2$$

and

$$\text{var}\,[y(\mathbf{X})] = \sum_{\emptyset \neq u \subseteq \{1,\ldots,N\}} \sum_{\mathbf{j}_u \in \mathbb{N}^{|u|}} C^2_{u,\mathbf{j}_u}.$$

Here, many terms of (27) and (28) associated with two unequal subsets u and v vanish as for independent variables $J_{u,\mathbf{j}_u;v,\mathbf{k}_v} = 0$ whenever $u \neq v$. The only summation terms retained are the ones when $u = v$ and $\mathbf{j}_u = \mathbf{k}_v$, resulting in $J_{u,\mathbf{j}_u;v,\mathbf{k}_v} = 1$.

Being convergent in probability and distribution, the probability density function of $y(\mathbf{X})$, if it exists, can also be estimated by that of $y_{S,m}(\mathbf{X})$. However, no analytical formula exists for the density function. In that case, the density can be estimated by sampling methods, such as MCS of $y_{S,m}(\mathbf{X})$. Such simulation should not be confused with crude MCS of $y(\mathbf{X})$, typically used for producing benchmark results whenever possible. The crude MCS can be expensive or even prohibitive, particularly when the sample size needs to be very large for estimating tail probabilistic characteristics. In contrast, the MCS applied to the GPDD approximation requires evaluations of simple polynomial functions that describe $y_{S,m}$. Therefore, a relatively large sample size can be accommodated in the GPDD approximation even when y is expensive to evaluate.

4.7. Numerical implementation

Algorithm 1 describes a procedure for developing an S-variate, mth-order GPDD approximation $y_{S,m}(\mathbf{X})$ of a general square-integrable function $y(\mathbf{X})$. It includes calculation of the mean and variance of $y_{S,m}(\mathbf{X})$.

Algorithm 1: GPDD approximation and second-moment statistics

Input: The total number N of input variables $\mathbf{X} = (X_1, \ldots, X_N)^T$, a joint probability density function $f_{\mathbf{X}}(\mathbf{x})$ of $\mathbf{X}$ satisfying Assumptions (1)–(4), a square-integrable function $y(\mathbf{X})$, and the largest degree of interaction S and largest order of orthogonal polynomials m

Output: The S-variate, mth-order GPDD approximation $y_{S,m}(\mathbf{X})$ of $y(\mathbf{X})$, mean and variance of $y_{S,m}(\mathbf{X})$

1 Calculate the marginal probability density functions $f_{\mathbf{X}_u}(\mathbf{x}_u)$ of $\mathbf{X}_u$ for all $1 \leq |u| \leq S$

2 **for** $l \leftarrow 1$ ***to*** m **do**

3 Generate the sets of orthogonal polynomials $\{P_{u,\mathbf{j}_u}(\mathbf{x}_u) : 1 \leq |u| \leq \min(S,l), |\mathbf{j}_u| = l\}$ and their standardized version $\{\Psi_{u,\mathbf{j}_u}(\mathbf{x}_u) : 1 \leq |u| \leq \min(S,l), |\mathbf{j}_u| = l\}$ that are consistent with the measure $f_{\mathbf{X}_u}(\mathbf{x}_u)d\mathbf{x}_u$
`/* from the Gram--Schmidt process or other means and (4) */`

4 Calculate or estimate $y_\emptyset$, $I_{u,\mathbf{j}_u}$, and $J_{u,\mathbf{j}_u;v,\mathbf{k}_v}$ for $1 \leq |u|, |v| \leq \min(S,l)$ and $|\mathbf{j}_u| = |\mathbf{k}_v| = l$
`/* from quasi MCS (QMCS) or other numerical methods */`

5 Construct and solve the linear system to obtain the lth-degree expansion coefficients $C_{u,\mathbf{j}_u}$, $1 \leq |u| \leq \min(S,l)$, $|\mathbf{j}_u| = l$
`/* from (25) */`

6 Compile the requisite set of S-variate, mth-order GPDD expansion coefficients and hence construct the S-variate, mth-order GPDD approximation $y_{S,m}(\mathbf{X})$
`/* from (19) */`

7 Calculate the mean $\mathbb{E}[y_{S,m}(\mathbf{X})]$ and variance $\text{var}[y_{S,m}(\mathbf{X})]$
`/* from (26) and (27) */`

5. Examples

Two examples, the one involving a stochastic ODE describing a three-dimensional diffusion problem and the other entailing 11-dimensional random eigenvalue problem from structural dynamics application, are presented to illustrate the proposed GPDD.

5.1. Stochastic ODE

Consider a stochastic boundary-value problem described by the ODE

$$-\frac{d}{d\xi}\left(\exp(X_1)\frac{d}{d\xi}y(\xi;\mathbf{X})\right) = (X_2+X_3)^2,\ 0 \leq \xi \leq 1,\ y(\xi;\mathbf{X}) \in \mathbb{R}, \tag{29}$$

Table 2
Three cases of input probability density functions.

Case	Probability density function
1	Gaussian density on $\mathbb{R}^3$: $f_{X_1X_2X_3}(x_1,x_2,x_3) = (2\pi)^{-\frac{3}{2}}(\det \mathbf{\Sigma_X})^{-\frac{1}{2}} \exp\left[-\frac{1}{2}\mathbf{x}^T\mathbf{\Sigma_X^{-1}}\mathbf{x}\right]$, $\mathbf{x} = (x_1,x_2,x_3)^T \in \mathbb{R}^3$, where $\Sigma_{\mathbf{X}} = \begin{bmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \rho_{13}\sigma_1\sigma_3 \\ & \sigma_2^2 & \rho_{23}\sigma_2\sigma_3 \\ (\text{sym.}) & & \sigma_3^2 \end{bmatrix}$, $\sigma_1 = \sigma_2 = \sigma_3 = 1/4$, $\rho_{12} = \rho_{13} = \rho_{23} = 1/5$.
2	Gegenbauer density on $\mathbb{B}^3$: $f_{X_1X_2X_3}(x_1,x_2,x_3) = \begin{cases} \frac{\Gamma(\mu+2)}{\pi^{\frac{3}{2}}\Gamma\left(\mu+\frac{1}{2}\right)}\left(1-\|\mathbf{x}\|^2\right)^{\mu-\frac{1}{2}}, & \mathbf{x} = (x_1,x_2,x_3)^T \in \mathbb{B}^3, \\ 0, & \text{otherwise}, \end{cases}$ where $\|\mathbf{x}\|^2 := \sum_{i=1}^{3} x_i^2$, $\mu = 5$.
3	Dirichlet density on $\mathbb{T}^3$: $f_{X_1X_2X_3}(x_1,x_2,x_3) = \begin{cases} \frac{\Gamma\left(\sum_{i=1}^{4}\kappa_i+2\right)}{\prod_{i=1}^{4}\Gamma\left(\kappa_i+\frac{1}{2}\right)}\left(\prod_{i=1}^{3}x_i^{\kappa_i-\frac{1}{2}}\right)(1-|\mathbf{x}|)^{\kappa_4-\frac{1}{2}}, & \mathbf{x} = (x_1,x_2,x_3)^T \in \mathbb{T}^3, \\ 0, & \text{otherwise}, \end{cases}$ where $\lvert\mathbf{x}\rvert := \sum_{i=1}^{3} x_i$, $\kappa_1 = \kappa_2 = \kappa_3 = \kappa_4 = 1$.

with boundary conditions

$$y(0;\mathbf{X}) = 0, \quad \exp(X_1)\frac{dy}{d\xi}(1;\mathbf{X}) = 1,$$

where $\mathbf{X} = (X_1, X_2, X_3)^T$ is a real-valued, trivariate input random vector with known probability density function. Three distinct cases of the probability density function of $\mathbf{X}$, one with an unbounded support and the other two with bounded supports, were considered: (1) a Gaussian density function on $\mathbb{R}^3 := \{(x_1,x_2,x_3) : -\infty < x_1,x_2,x_3 < +\infty\}$; (2) a Gegenbauer density function on the unit disk $\mathbb{B}^3 := \{(x_1,x_2,x_3) : x_1^2+x_2^2+x_3^2 \le 1\}$; and (3) a Dirichlet density function on the standard tetrahedron $\mathbb{T}^3 := \{(x_1,x_2,x_3) : 0 \le x_1,x_2,x_3; x_1+x_2+x_3 \le 1\}$. Table 2 presents explicit forms of the density functions, including the values of their parameters. For all three cases, a three-dimensional contour plot of the joint density $f_{X_1X_2X_3}(x_1,x_2,x_3) = 0$ (left) and several contours of $f_{X_1X_2X_3}(x_1,x_2,x_3)$ over slice planes through the center (right) are depicted in Figs. 2(a), 3(a), and 4(a). The marginal densities of (X_i, X_j) (left) and X_i (right), $i, j = 1,2,3$ $i \neq j$, are drawn in Figs. 2(b), 3(b), and 4(b). The objective is to assess the approximation quality of the truncated GPDD in terms of the second-moment statistics of the solution of the ODE.

5.1.1. Orthogonal polynomials

The aforementioned input density functions satisfy Assumptions (1) and (2). Therefore, measure-consistent orthogonal polynomial bases exist in all cases. However, there are multiple and explicit forms of orthogonal polynomial bases [19]. In this work, however, a set of orthogonal polynomials $\{P_{u,\mathbf{j}_u}(\mathbf{x}_u)\colon 1 \le |u| \le 3, |u| \le |\mathbf{j}_u| \le 6\}$, consistent with the Gaussian, Gegenbauer, and Dirichlet density functions, were determined using the respective formulae described in Section 3.5. They were later scaled using (4) to generate their standardized version $\{\Psi_{u,\mathbf{j}_u}(\mathbf{x}_u)\}$. More explicitly, Table 3 presents first-, second-, and third-order (-degree) orthogonal polynomials in $\mathbf{x}_u$, $1 \le |u| \le 3$, obtained for all three density functions; here, the indices $i = 1,2,3$ and $i_1, i_2 = 1,2,3$, $i_2 > i_1$. It is easy to verify

Table 3
A few orthogonal polynomials consistent with the three density functions of Example 1.[a]

Case 1: Gaussian density on $\mathbb{R}^3$ ($\sigma_1=\sigma_2=\sigma_3=1/4,\ \rho_{12}=\rho_{13}=\rho_{23}=1/5$)

$$\Psi_{\{i\}1}=4x_i,$$

$$\Psi_{\{i\}2}=8\sqrt{2}x_i^2-\tfrac{1}{\sqrt{2}},$$

$$\Psi_{\{i\}3}=32\sqrt{\tfrac{2}{3}}x_i^3-2\sqrt{6}x_i,$$

$$\Psi_{\{i_1,i_2\}11}=-\tfrac{25}{3}\sqrt{\tfrac{2}{13}}x_{i_1}^2+\tfrac{10}{3}\sqrt{26}x_{i_2}x_{i_1}-\tfrac{25}{3}\sqrt{\tfrac{2}{13}}x_{i_2}^2+\tfrac{1}{\sqrt{26}},$$

$$\Psi_{\{i_1,i_2\}12}=\tfrac{50x_{i_1}^3}{27}-\tfrac{170}{9}x_{i_2}x_{i_1}^2+50x_{i_2}^2x_{i_1}-3x_{i_1}-\tfrac{250x_{i_2}^3}{27}+\tfrac{5x_{i_2}}{3},$$

$$\Psi_{\{i_1,i_2\}21}=-\tfrac{250x_{i_1}^3}{27}+50x_{i_2}x_{i_1}^2-\tfrac{170}{9}x_{i_2}^2x_{i_1}+\tfrac{5x_{i_1}}{3}+\tfrac{50x_{i_2}^3}{27}-3x_{i_2},$$

$$\begin{aligned}\Psi_{\{1,2,3\}111}=&\tfrac{60}{7}\sqrt{\tfrac{10}{203}}x_1^3-\tfrac{310}{7}\sqrt{\tfrac{10}{203}}x_2x_1^2-\tfrac{310}{7}\sqrt{\tfrac{10}{203}}x_3x_1^2-\tfrac{310}{7}\sqrt{\tfrac{10}{203}}x_2^2x_1-\tfrac{310}{7}\sqrt{\tfrac{10}{203}}x_3^2x_1\\&+\tfrac{80}{7}\sqrt{\tfrac{290}{7}}x_2x_3x_1+2\sqrt{\tfrac{10}{203}}x_1+\tfrac{60}{7}\sqrt{\tfrac{10}{203}}x_2^3+\tfrac{60}{7}\sqrt{\tfrac{10}{203}}x_3^3-\tfrac{310}{7}\sqrt{\tfrac{10}{203}}x_2x_3^2\\&+2\sqrt{\tfrac{10}{203}}x_2-\tfrac{310}{7}\sqrt{\tfrac{10}{203}}x_2^2x_3+2\sqrt{\tfrac{10}{203}}x_3.\end{aligned}$$

Case 2: Gegenbauer density on the unit ball $\mathbb{B}^3$ ($\mu=5$)

$$\Psi_{\{i\}1}=-\sqrt{14}x_i,$$

$$\Psi_{\{i\}2}=28\sqrt{\tfrac{2}{13}}x_i^2-2\sqrt{\tfrac{2}{13}},$$

$$\Psi_{\{i\}3}=3\sqrt{\tfrac{42}{13}}x_i-16\sqrt{\tfrac{42}{13}}x_i^3,$$

$$\Psi_{\{i_1,i_2\}11}=4\sqrt{14}x_{i_1}x_{i_2},$$

$$\Psi_{\{i_1,i_2\}12}=-2\sqrt{\tfrac{42}{13}}x_{i_1}^3-2\sqrt{546}x_{i_2}^2x_{i_1}+2\sqrt{\tfrac{42}{13}}x_{i_1},$$

$$\Psi_{\{i_1,i_2\}21}=-2\sqrt{\tfrac{42}{13}}x_{i_2}^3-2\sqrt{546}x_{i_1}^2x_{i_2}+2\sqrt{\tfrac{42}{13}}x_{i_2},$$

$$\Psi_{\{123\}111}=-24\sqrt{7}x_1x_2x_3.$$

Case 3: Dirichlet density on the standard tetrahedron $\mathbb{T}^3$ ($\kappa_1=\kappa_2=\kappa_3=\kappa_4=1$)

$$\Psi_{\{i\}1}=\sqrt{\tfrac{7}{3}}-4\sqrt{\tfrac{7}{3}}x_i,$$

$$\Psi_{\{i\}2}=\tfrac{224x_i^2}{\sqrt{55}}-28\sqrt{\tfrac{5}{11}}x_i+3\sqrt{\tfrac{5}{11}},$$

$$\Psi_{\{i\}3}=-128\sqrt{\tfrac{15}{13}}x_i^3+672\sqrt{\tfrac{3}{65}}x_i^2-112\sqrt{\tfrac{5}{39}}x_i+7\sqrt{\tfrac{5}{39}},$$

$$\Psi_{\{i_1,i_2\}11}=11\sqrt{\tfrac{42}{19}}x_{i_1}^2+2\sqrt{798}x_{i_2}x_{i_1}-14\sqrt{\tfrac{42}{19}}x_{i_1}+11\sqrt{\tfrac{42}{19}}x_{i_2}^2-14\sqrt{\tfrac{42}{19}}x_{i_2}+3\sqrt{\tfrac{42}{19}},$$

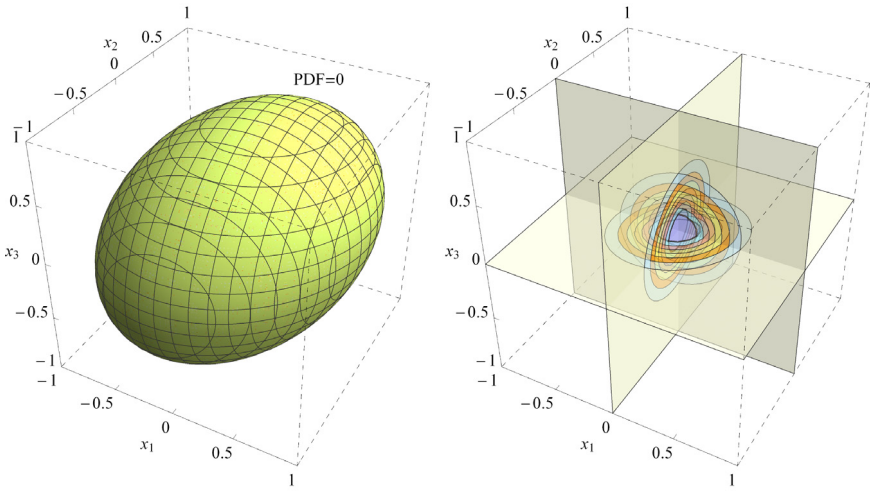
$$\begin{aligned}\Psi_{\{i_1,i_2\}12}=&-6\sqrt{\tfrac{1001}{37}}x_{i_1}^3-614\sqrt{\tfrac{77}{481}}x_{i_2}x_{i_1}^2+174\sqrt{\tfrac{77}{481}}x_{i_1}^2-2\sqrt{37037}x_{i_2}^2x_{i_1}+788\sqrt{\tfrac{77}{481}}x_{i_2}x_{i_1}\\&-114\sqrt{\tfrac{77}{481}}x_{i_1}-18\sqrt{\tfrac{1001}{37}}x_{i_2}^3+30\sqrt{\tfrac{1001}{37}}x_{i_2}^2-174\sqrt{\tfrac{77}{481}}x_{i_2}+18\sqrt{\tfrac{77}{481}},\end{aligned}$$

$$\begin{aligned}\Psi_{\{i_1,i_2\}21}=&-18\sqrt{\tfrac{1001}{37}}x_{i_1}^3-2\sqrt{37037}x_{i_2}x_{i_1}^2+30\sqrt{\tfrac{1001}{37}}x_{i_1}^2-614\sqrt{\tfrac{77}{481}}x_{i_2}^2x_{i_1}+788\sqrt{\tfrac{77}{481}}x_{i_2}x_{i_1}\\&-174\sqrt{\tfrac{77}{481}}x_{i_1}-6\sqrt{\tfrac{1001}{37}}x_{i_2}^3+174\sqrt{\tfrac{77}{481}}x_{i_2}^2-114\sqrt{\tfrac{77}{481}}x_{i_2}+18\sqrt{\tfrac{77}{481}},\end{aligned}$$

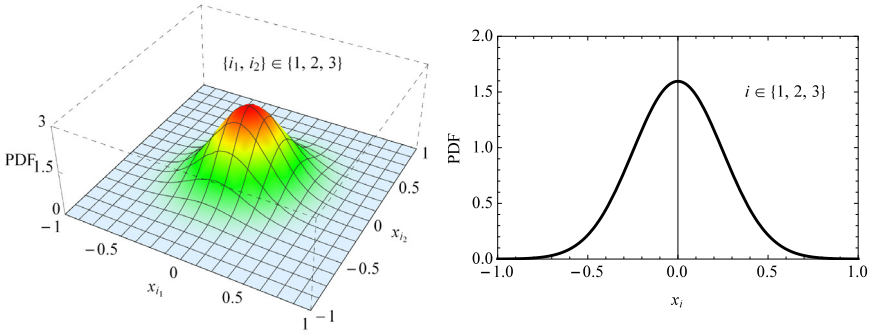
$$\begin{aligned}\Psi_{\{1,2,3\}111}=&-12\sqrt{55}x_1^3-50\sqrt{55}x_2x_1^2-50\sqrt{55}x_3x_1^2+138\sqrt{\tfrac{11}{5}}x_1^2-50\sqrt{55}x_2^2x_1-50\sqrt{55}x_3^2x_1\\&+346\sqrt{\tfrac{11}{5}}x_2x_1-128\sqrt{55}x_2x_3x_1+346\sqrt{\tfrac{11}{5}}x_3x_1-96\sqrt{\tfrac{11}{5}}x_1-12\sqrt{55}x_2^3\\&-12\sqrt{55}x_3^3+138\sqrt{\tfrac{11}{5}}x_2^2-50\sqrt{55}x_2x_3^2+138\sqrt{\tfrac{11}{5}}x_3^2-96\sqrt{\tfrac{11}{5}}x_2-50\sqrt{55}x_2^2x_3\\&+346\sqrt{\tfrac{11}{5}}x_2x_3-96\sqrt{\tfrac{11}{5}}x_3+18\sqrt{\tfrac{11}{5}}.\end{aligned}$$

[a] Here, $i=1,2,3$; $i_1,i_2=1,2,3$, $i_2>i_1$.

from (6) and (7) that all polynomials of Table 3 have *zero* means and any two distinct polynomials are orthogonal whenever ($u\subset v\subset u, \forall\, \mathbf{j}_u, \mathbf{k}_v$) or ($\forall\, u, v, |\mathbf{j}_u|\neq|\mathbf{k}_v|$).



(a)



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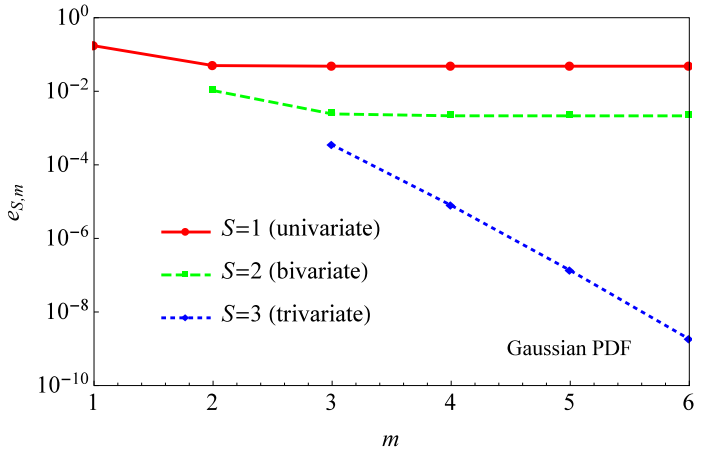
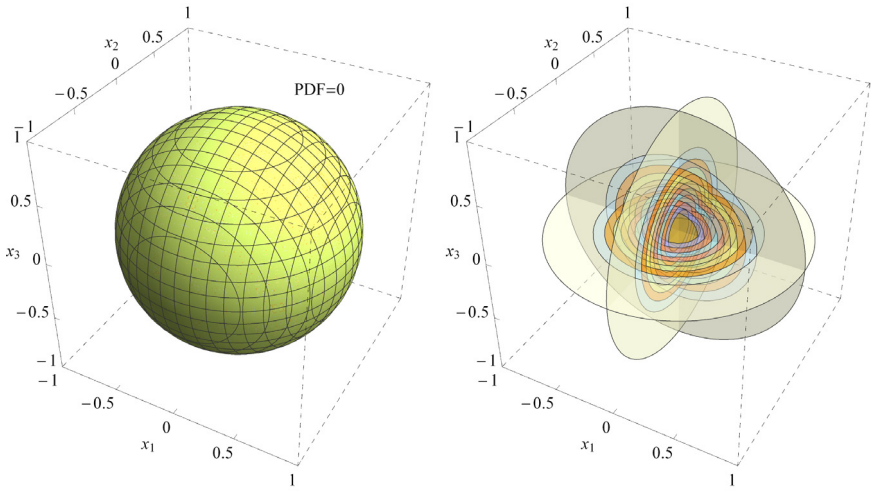
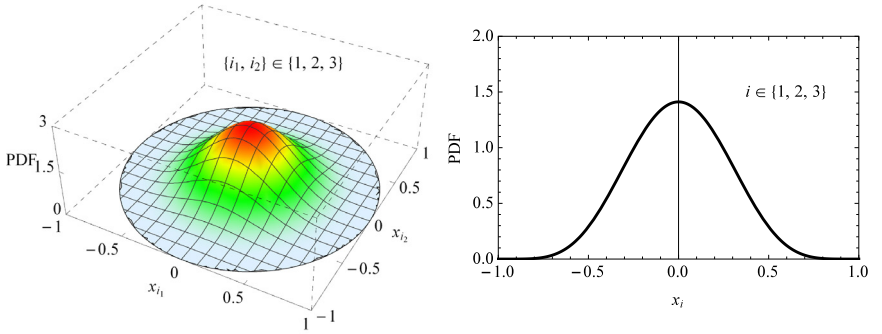


(c)

Fig. 2. Input probability measures and GPDD results for the Gaussian density on $\mathbb{R}^3$; (a) contour plot of $f_{X_1X_2X_3}(x_1, x_2, x_3) = 0$ (left) and sliced contours of $f_{X_1X_2X_3}(x_1, x_2, x_3)$ (right); (b) marginal densities of (X_i, X_j) (left) and X_i (right); (c) decay of L^1 error in the variance of $y_{S,m}(1; \mathbf{X})$ with respect to m.



(a)



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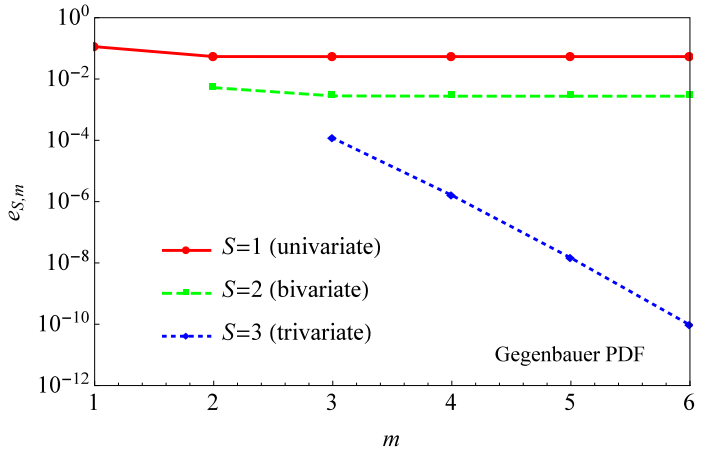
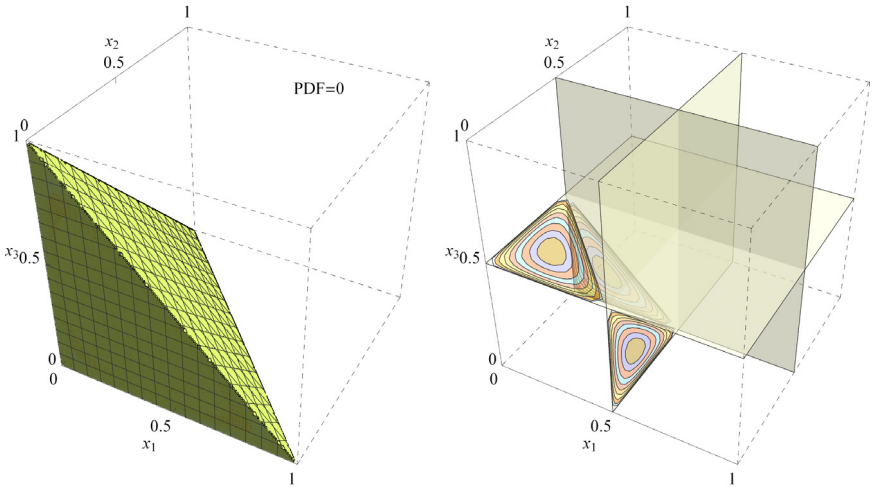
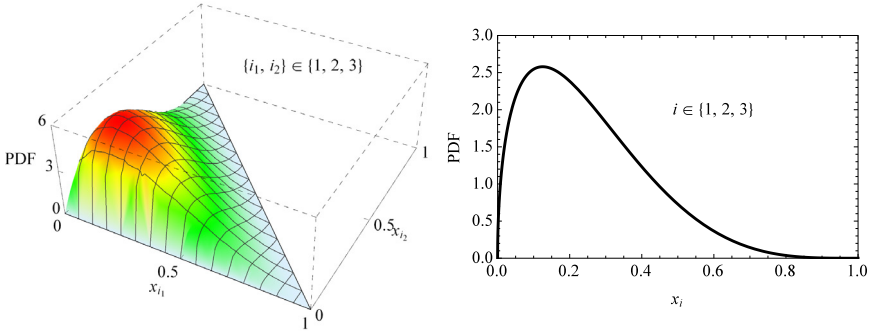


(c)

Fig. 3. Input probability measures and GPDD results for the Gegenbauer density on $\mathbb{B}^3$; (a) contour plot of $f_{X_1X_2X_3}(x_1, x_2, x_3) = 0$ (left) and sliced contours of $f_{X_1X_2X_3}(x_1, x_2, x_3)$ (right); (b) marginal densities of (X_i, X_j) (left) and X_i (right); (c) decay of L^1 error in the variance of $y_{S,m}(1; \mathbf{X})$ with respect to m.



(a)



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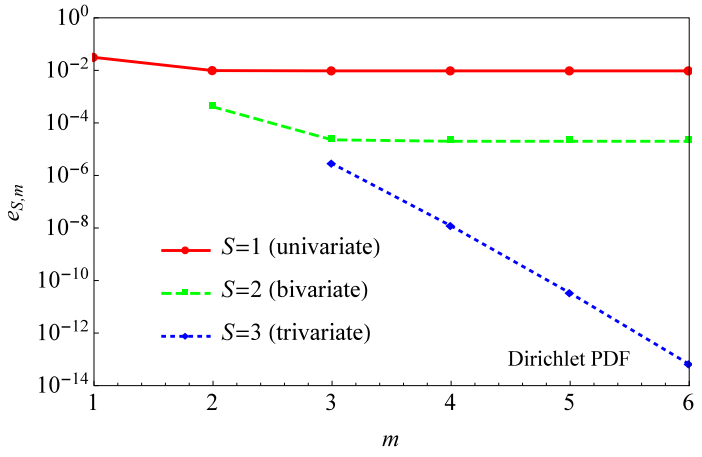


(c)

Fig. 4. Input probability measures and GPDD results for the Dirichlet density on $\mathbb{T}^3$; (a) contour plot of $f_{X_1X_2X_3}(x_1, x_2, x_3) = 0$ (left) and sliced contours of $f_{X_1X_2X_3}(x_1, x_2, x_3)$ (right); (b) marginal densities of (X_i, X_j) (left) and X_i (right); (c) decay of L^1 error in the variance of $y_{S,m}(1; \mathbf{X})$ with respect to m.

5.1.2. Exact solution

A straightforward integration of (29) leads to the exact solution:

$$y(\xi;\mathbf{X}) = \frac{1}{\exp(X_1)}\left[\xi + \left(\xi - \frac{\xi^2}{2}\right)(X_2+X_3)^2\right]. \tag{30}$$

Clearly, the first two raw moments $\mathbb{E}[y(\xi;\mathbf{X})]$ and $\mathbb{E}[y^2(\xi;\mathbf{X})]$, or any probabilistic characteristics of $y(\xi;\mathbf{X})]$ for that matter, depend on the probability density of $\mathbf{X}$. Appendix B provides analytical results of these two moments at $\xi = 1$ for all three cases of input density functions.

5.1.3. GPDD solution

The Gaussian density function, which has an unbounded support, satisfies Assumption (3b) [25], whereas the density functions on the unit ball and the standard tetrahedron, which have bounded supports, clearly fulfill Assumption (3a). Moreover, the support of each density function is grid-closed for the parameters chosen, that is, Assumption (4) is also satisfied. Furthermore, $y(\xi;\mathbf{X})$ is a square-integrable function. Therefore, GPDD can be applied to solve this problem for all three density functions. However, since $y(\xi;\mathbf{X})$ is a non-polynomial function of $\mathbf{X}$, a convergence analysis with respect to m – the order of GPDD approximation –is essential. Employing $S = 1, 2, 3$ and $m = 1, 2, 3, 4, 5, 6$, various GPDD approximations of $y(\xi;\mathbf{X})$ and their second-moment statistics were constructed or calculated for all three density functions.

Define at $\xi = 1$ an L^1 error

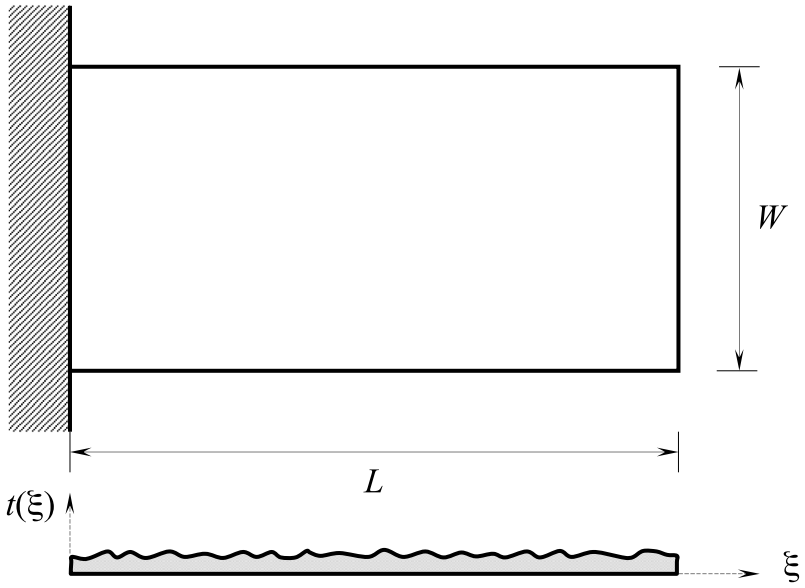
$$e_{S,m} := \frac{\left|\text{var}[y(1;\mathbf{X})] - \text{var}[y_{S,m}(1;\mathbf{X})]\right|}{\text{var}[y(1;\mathbf{X})]} \tag{31}$$

in the variance, committed by an S-variate, mth-order GPDD approximation $y_{S,m}(1;\mathbf{X})$ of $y(1;\mathbf{X})$, where $\text{var}[y(1;\mathbf{X})]$ and $\text{var}[y_{S,m}(1;\mathbf{X})]$ are exact and approximate variances, respectively. The exact variance was obtained from the first two raw moments in (B.1) through (B.6), depending on the input probability measure, whereas the approximate variance, given S and m, was calculated following (27). The integrals $I_{u,\mathbf{j}_u}$ and $J_{u,\mathbf{j}_u;v,\mathbf{k}_v}$, needed to determine the expansion coefficients $C_{u,\mathbf{j}_u}$ and $y_\emptyset$, were calculated analytically for all three density functions. Therefore, the variances from the GPDD approximations and resultant errors were determined exactly.

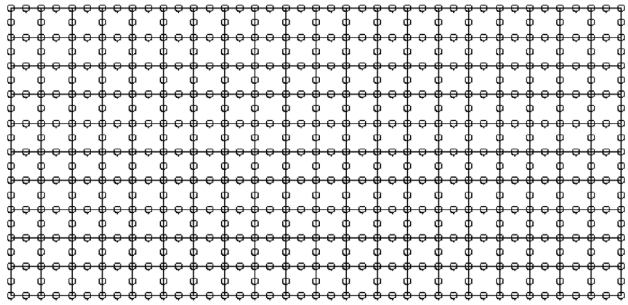
Fig. 2(c) presents three plots describing how the error $e_{S,m}$ of a GPDD approximation in (31), obtained using the Gaussian density function of input variables, decays with respect to m. The three plots correspond to three GPDD truncations with respect to the degree of interaction $S = 1$ (univariate), $S = 2$ (bivariate), and $S = 3$ (trivariate). In all cases, the approximation errors drop with respect to S and m as expected. In addition, the errors committed by the univariate and bivariate GPDD approximations may decline further by increasing m, but they level off at respective limits. The magnitudes of how much they decline and their limits depend on the function y and are expected to be more pronounced if y is a highly nonlinear function of $\mathbf{X}$, but endowed with no or little interactions among input variables. In contrast, the errors from the trivariate GPDD approximation do not settle down, descend strictly monotonically with respect to m, and lead to nearly exponential convergence. This is because in the trivariate approximation S is equal to three, the total number (N) of random variables in this problem. Similar plots of error analysis obtained using the Gegenbauer and Dirichlet density functions are displayed in Fig. 3(c) and Fig. 4(c), respectively. The results are qualitatively the same as those discussed for the case of Gaussian density function.

5.2. Random eigenvalue problem

The final example entails random eigenvalue analysis of an undamped cantilever plate, shown in Fig. 5(a), often performed in structural dynamics. The plate has the following deterministic geometric and material properties: length $L = 2$ in (50.8 mm), width $W = 1$ in (25.4 mm), Young's modulus $E = 30 \times 10^6$ psi (206.8 GPa), Poisson's ratio $\nu = 0.3$, and mass density $\rho = 7.324 \times 10^{-4}$ lb-s^2/in^4 (7827 kg/mm^3). The randomness in eigenvalues arises due to random thickness $t(\xi)$, which is spatially varying in the longitudinal direction ξ only. The thickness is represented by a homogeneous, lognormal random field $t(\xi) = c\exp[\alpha(\xi)]$ with mean $\mu_t = 0.01$ in (0.254 mm), variance $\sigma_t^2 = v_t^2\mu_t^2$, and coefficient of variation $v_t = 0.2$, where $c = \mu_t/\sqrt{1+v_t^2}$ and $\alpha(\xi)$ is a zero-mean, homogeneous, Gaussian random field with variance $\sigma_\alpha^2 = \ln(1+v_t^2)$ and covariance function $\Gamma_\alpha(\tau) = \mathbb{E}[\alpha(\xi)\alpha(\xi+\tau) = \sigma_\alpha^2\exp[-|\tau|/(0.2L)]$. Two numerical grids were employed: (1) a 10×20 finite-element grid of the plate, consisting of 200 eight-noded,



(a)



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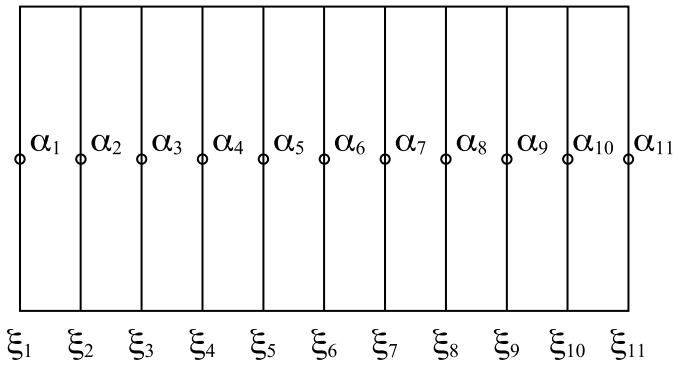

(c)

Fig. 5. A cantilever plate; (a) geometry; (b) finite-element grid; (c) random-field grid.

Table 4
Second-moment properties of the first four eigenvalues of the cantilever plate by three GPDD approximations and crude MCS.

	Univariate, 1st-order GPDD		Univariate, 2nd-order GPDD		Bivariate, 2nd-order GPDD		Crude MCS (10,000 samples)	
Λ[a]	Mean	St. dev.	Mean	St. dev.	Mean	St. dev.	Mean	St. dev.
Λ_1	0.275088	0.0869715	0.275088	0.0880851	0.275088	0.0896882	0.274852	0.0888108
Λ_2	5.10714	1.18771	5.10714	1.19738	5.10714	1.21458	5.10376	1.20242
Λ_3	10.6004	2.0924	10.6004	2.10071	10.6004	2.14212	10.5987	2.14294
Λ_4	54.5265	9.85134	54.5265	9.90945	54.5265	10.1103	54.5506	10.0225

[a] The unit of eigenvalue is $(\text{rad/ms})^2$.

second-order shell elements and 661 nodes, as shown in Fig. 5(b); and (2) an 11-point random-field grid of the plate, parameterizing the random field $\alpha(\xi)$ into a zero-mean, 11-dimensional, dependent Gaussian random vector $\mathbf{X} = (\alpha_1, \ldots, \alpha_{11})^T$ with covariance matrix $\mathbf{\Sigma_X} = [\Gamma_\alpha(\xi_i - \xi_j)]$, $i, j = 1, \ldots, 11$, where ξ_i is the coordinate of the column of nodes after traversing $2(i-1)$ columns of finite elements from the left, as shown in Fig. 5(c). The thickness is linearly interpolated between two consecutive nodes of the random-field grid. The finite-element grid was used for domain discretization, generating the random mass matrix $\mathbf{M(X)}$ and random stiffness matrix $\mathbf{K(X)}$ of the cantilever plate. The random eigenvalue problem calls for solving the matrix characteristic equation: $\det[\mathbf{K(X)} - \mathbf{\Lambda(X)M(X)}] = 0$, where $\mathbf{\Lambda(X)}$ is a random eigenvalue of interest with its square-root representing the corresponding natural frequency. A Lanczos algorithm [33] was used to calculate the eigenvalue.

Three GPDD approximations described by (19) were employed to estimate various probabilistic characteristics of the first four eigenvalues of the plate: (1) univariate, first-order GPDD approximation ($S = 1$, $m = 1$), (2) univariate, second-order GPDD approximation ($S = 1$, $m = 2$), and (3) bivariate, second-order GPDD approximation ($S = 2$, $m = 2$). All univariate and bivariate orthogonal polynomials involved were exactly determined by analytical formula as before. However, unlike in the former example, $I_{u,\mathbf{j}_u}$ and $J_{u,\mathbf{j}_u;v,\mathbf{k}_v}$, needed to calculate the expansion coefficients $C_{u,\mathbf{j}_u}$ and $y_\emptyset$, are all 11-dimensional integrals entailing an implicit function from FEA, and hence, they cannot be determined exactly. Instead, a QMCS [34] was used to estimate the integrals, yielding approximate coefficients in three steps: (1) select a QMCS sample size $L_{QMCS} \in \mathbb{N}$ and generate a low-discrepancy point set $\mathcal{P}_{L_{QMCS}} := \{\mathbf{u}^{(k)} \in [0,1]^{11}, k = 1, \ldots, L_{QMCS}\}$; (2) map each sample from $\mathcal{P}_{L_{QMCS}}$ to the sample $\mathbf{x}^{(k)} \in \mathbb{R}^{11}$, following the Gaussian probability measure of $\mathbf{X}$; and (3) approximate the integrals as arithmetic averages of integrand values at the aforementioned point set. The computational cost of QMCS is proportional to L_{QMCS}, as all sample calculations require the same effort. The Sobol sequence [35] was used for the low-discrepancy point set with the value of $L_{QMCS} = 3000$. The sample size chosen was deemed adequate for this problem.

5.2.1. Second-moment statistics

Table 4 presents the means and standard deviations of the first four eigenvalues, Λ_i, $i = 1, \ldots, 4$, of the plate by four different methods: the three GPDD approximations and crude MCS. In all four methods, the solution of the matrix characteristic equation for a given input is equivalent to performing an FEA. Therefore, computational efficiency, even for this simple plate, is a practical requirement in solving random eigenvalue problems. Due to the expense of FEA, crude MCS was conducted for a sample size $L_{MCS} = 10{,}000$, which should be adequate for providing benchmark solutions of the second-moment characteristics. The agreement between the means and standard deviations by all three GPDD approximations and crude MCS in Table 4 is generally good. However, the univariate, second-order and bivariate, second-order GPDD approximations are relatively more accurate than the univariate, first-order GPDD approximation in estimating standard deviations, as expected.

5.2.2. Cumulative distribution function

Fig. 6 illustrates the marginal cumulative distribution functions, respectively, of the four eigenvalues by the three GPDD approximations and crude MCS. Due to the computational expense inherent to FEA, the same 10,000 samples generated for verifying the statistics in Table 4 were utilized for the crude MCS estimates in Fig. 6. However, since the GPDD approximations yield explicit eigenvalue approximations in terms of multivariate polynomials, a relatively large sample size, 100,000 in this particular example, was selected to sample (19) for estimating the

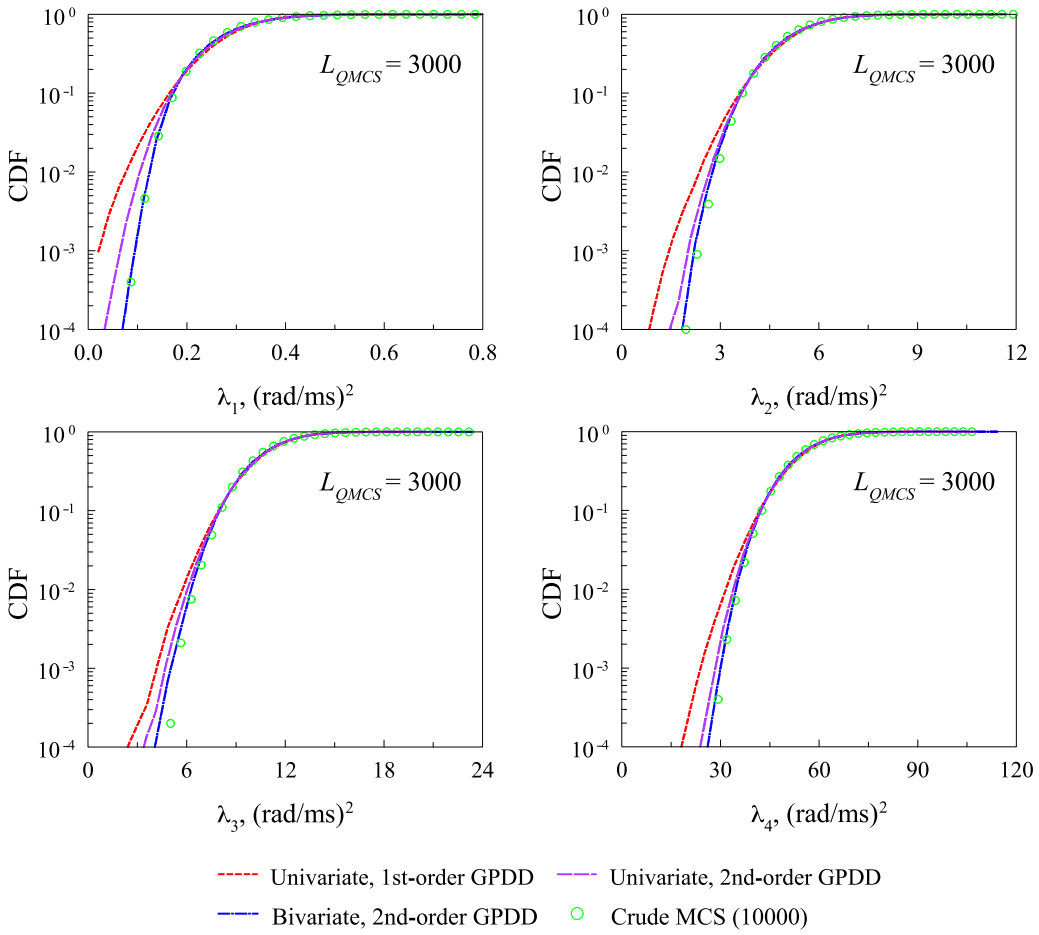

Fig. 6. Marginal cumulative distribution functions (CDFs) of the first four eigenvalues of the cantilever plate by three GPDD approximations and crude MCS.

respective distribution functions. According to Fig. 6, the distribution functions estimated by the bivariate, second-order GPDD approximations and crude MCS match extremely well over the entire support for all four eigenvalues. In contrast, the univariate, first-order GPDD approximations produce satisfactory estimates of distribution functions only around the means or medians; however, in the tail regions there are significant discrepancies. This is because of the lack of interactions among and/or nonlinear effects of input variables in a low-order univariate approximation. Interestingly, the distribution functions from the univariate, second-order GPDD approximations are close to those from the bivariate, second-order GPDD approximations or crude MCS, thereby producing palpably improved results. This is possible as a higher-order univariate approximation can capture arbitrarily large nonlinear behavior of the response, although it cannot pick up any interactive effects of input variables.

In closing this section, a brief discussion on the practical significance of the work is warranted. First and foremost, GPDD acquires the desirable hierarchical structure of the generalized ADD, and is, therefore, expected to ameliorate the curse of dimensionality to the extent possible in tackling a high-dimensional UQ problem. By removing the independence assumption, GPDD opens a new avenue for treatment of dependent random variables and should be able to solve large-scale UQ problems subject to more realistic input distributions than before. Second, the GPDD method entailing polynomials, orthogonal with respect to the original, non-product-type probability density function, is expected to converge faster than the commonly used tensor product PDD method in the transformed variables. This is because the measure transformations – with the exception of dependent Gaussian variables, where such transformations are linear – often lead to highly nonlinear output functions of transformed variables. Third, the

GPDD proposed is particularly beneficial for non-trivial domains, such as a ball or a simplex, where *a priori* measure transformations are complicated or impractical. Fourth, stable formulae for computing measure-consistent orthogonal polynomials, at least for the special cases considered in the paper, are highly desirable.

6. Future work

While this paper has presented a novel approach for tackling dependent random variables, there remain two outstanding computational challenges for future endeavors. First, the calculation of the expansion coefficients of the GPDD method requires evaluating various N-dimensional integrals $I_{u,\mathbf{j}_u}$, $J_{u,\mathbf{j}_u;v,\mathbf{k}_v}$, and $y_\emptyset$ on $\mathbb{A}^N$, which cannot be determined analytically or exactly if y is a general function and $f_{\mathbf{X}}(\mathbf{x})d\mathbf{x}$ is a general probability measure. Furthermore, for large N, a full numerical integration employing an N-dimensional tensor product of a univariate quadrature formula is computationally expensive and likely prohibitive. In Section 5, a QMCS was employed to estimate these integrals. However, in the future, more efficient alternative methods, such as sparse-grid quadrature [6], dimension-reduction integration [36], and other numerical methods, should be pursued or developed for calculating these integrals. Denote by $\tilde{I}_{u,\mathbf{j}_u}$, $\tilde{J}_{u,\mathbf{j}_u;v,\mathbf{k}_v}$, and $\tilde{y}_\emptyset$ the estimates of the aforementioned integrals from an approximate method of choice. Therefore, instead of (25), the actual finite-dimensional linear system involving approximate coefficients $\tilde{C}_{u,\mathbf{j}_u}$, $1 \le |u| \le \min(S,l)$ and $|\mathbf{j}_u| = l$, is

$$\sum_{\substack{\emptyset \neq v \subseteq \{1,\ldots,N\} \\ 1 \le |v| \le \min(S,l)}} \sum_{\substack{\mathbf{k}_v \in \mathbb{N}^{|v|} \\ |\mathbf{k}_v| = |\mathbf{j}_u|}} \tilde{C}_{v,\mathbf{k}_v} \tilde{J}_{u,\mathbf{j}_u;v,\mathbf{k}_v} = \tilde{I}_{u,\mathbf{j}_u}, \ 1 \le |u| \le \min(S,l), \ |\mathbf{j}_u| = l, \tag{32}$$

which is ready to be implemented and solved, and is scalable to higher dimensions in a straightforward way. Once the linear system (32) is solved for all $1 \le l \le m$, the result is a truly implementable S-variate, mth-order GPDD approximation

$$\tilde{y}_{S,m}(\mathbf{X}) = \tilde{y}_\emptyset + \sum_{\substack{\emptyset \neq u \subseteq \{1,\ldots,N\} \\ 1 \le |u| \le S}} \sum_{\substack{\mathbf{j}_u \in \mathbb{N}^{|u|} \\ |u| \le |\mathbf{j}_u| \le m}} \tilde{C}_{u,\mathbf{j}_u} \Psi_{u,\mathbf{j}_u}(\mathbf{X}_u)$$

of $y(\mathbf{X})$ for a general UQ problem.

Second, multivariate orthogonal polynomials in $\mathbf{x}_u$ consistent with the input probability measure must be generated. For Gaussian density on $\mathbb{R}^{|u|}$ and select densities on the unit ball $\mathbb{B}^{|u|}$ or the standard simplex $\mathbb{T}^{|u|}$, measure-consistent orthogonal polynomials can be generated analytically, as explained in Section 3.5. Therefore, measure-consistent orthogonal polynomials for these probability measures can be produced purely analytically. However, for general probability measures, no such analytical solutions exist; instead, numerical approximations are required. For instance, the Gram–Schmidt process can be employed to generate from monomials a sequence of orthogonal polynomials. However, the process is known to be ill-conditioned. Therefore, more stable methods are needed to compute orthogonal polynomials. Moreover, deriving an analytical formula for the second-moment properties of orthogonal polynomials for arbitrary non-Gaussian measures is nearly impossible. Having said so, these properties, which represent high-dimensional integrals comprising products of orthogonal polynomials, can be determined by writing them as a sum of expectations of monomials $\{\mathbf{X}^{\mathbf{j}}\}$, $0 \le |\mathbf{j}| \le 2m$, where the moments of $\mathbf{X}$ are calculated either analytically, if possible, or by numerical integration. Note that the numerical integration can be performed with an arbitrary precision even when N is large. This is because no generally expensive output function evaluations are involved.

7. Conclusion

A new computational method, referred to as the GPDD method, is presented for UQ analysis of complex systems subject to dependent input random variables. The method involves a Fourier-like series expansion of a high-dimensional random output function in terms of a hierarchically ordered, measure-consistent multivariate orthogonal polynomials in dependent input variables. The proposed GPDD, which can be viewed as a generalized version of the existing PDD, exists for any square-integrable function and converges in mean-square to the correct limit, provided that a few assumptions on the input probability measures are met. The GPDD method does not require independence of random variables; yet, it generates a convergent sequence of low-variate, low-order approximations for efficiently estimating the probabilistic characteristics of a general stochastic response of interest. New formulae are

developed to calculate the mean and variance of a GPDD approximation of a general output variable in terms of the expansion coefficients and second-moment properties of multivariate orthogonal polynomials. However, unlike in the existing PDD, calculating the coefficients of GPDD requires solving a coupled system of linear equations. Moreover, the variance formula of GPDD contains additional terms – a consequence of statistical dependence among input random variables – that are not present in that of PDD. The additional terms vanish as they should when the input variables are statistically independent, regressing the proposed PDD to the existing PDD. Two UQ problems – the one involving a stochastic ODE from three-dimensional diffusion analysis and the other entailing an 11-dimensional random eigenvalue analysis from structural dynamics – were solved, illustrating the construction and use of GPDD approximations in estimating various statistical properties of output variables.

Appendix A. Annihilating conditions revisited

Proposition 3. *Let $f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\alpha}_u)$, $\emptyset \neq u \subseteq \{1,\ldots,N\}$, be an infinitely differentiable probability density function of $\mathbf{X}_u := (X_{i_1},\ldots,X_{i_{|u|}})^T$. Denote by $\{P_{u,\mathbf{j}_u}(\mathbf{x}_u) : \mathbf{j}_u \in \mathbb{N}^N\}$ an infinite set of multivariate orthogonal polynomials, which are generated using the formula (10). Assume that the density function is either compactly supported or it converges to zero faster than the rate at which the polynomials become unbounded at the boundary. Then each multivariate orthogonal polynomial of the set satisfies the weak annihilating conditions (5).*

Proof. Let $\emptyset \neq u \subseteq \{1,\ldots,N\}$, $\mathbf{j}_u \in \mathbb{N}^N$, and $i \in u$. Then

$$
\begin{aligned}
&\int_{\mathbb{A}^{\{i\}}} P_{u,\mathbf{j}_u}(\mathbf{x}_u) f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\alpha}_u) dx_i \\
&\propto \int_{\mathbb{A}^{\{i\}}} \left(\frac{\partial}{\partial \mathbf{x}_u}\right)^{\mathbf{j}_u} f_{\mathbf{X}_u}(\mathbf{x}_u;\boldsymbol{\beta}_u) dx_i \\
&= \int_{\mathbb{A}^{\{i\}}} \frac{\partial^{j_{i_1},\ldots,j_{i_{|u|}}}}{\partial x_{i_1}^{j_{i_1}} \cdots x_{i_{|u|}}^{j_{i_{|u|}}}} \left\{ f_{\mathbf{X}_u}(x_{i_1},\ldots,x_{i_{|u|}};\boldsymbol{\beta}_u)\right\} dx_i \\
&= \left[\frac{\partial^{j_{i_1},\ldots,(j_i-1),\ldots,j_{i_{|u|}}}}{\partial x_{i_1}^{j_{i_1}} \cdots x_i^{(j_i-1)} \cdots x_{i_{|u|}}^{j_{i_{|u|}}}} \left\{ f_{\mathbf{X}_u}(x_{i_1},\ldots,x_i,\ldots,x_{i_{|u|}};\boldsymbol{\beta}_u)\right\} \right]_{\partial\mathbb{A}^{\{i\}}} \\
&= \Big[P_{\{i_1,\ldots,i,\ldots,i_{|u|}\},(j_{i_1},\ldots,(j_i-1),\ldots,j_{i_{|u|}})}(x_{i_1},\ldots,x_i,\ldots,x_{i_{|u|}}) \times \\
&\quad f_{\mathbf{X}_u}(x_{i_1},\ldots,x_i,\ldots,x_{i_{|u|}};\boldsymbol{\beta}_u)\Big]_{\partial\mathbb{A}^{\{i\}}} \\
&= 0.
\end{aligned}
\tag{A.1}
$$

Here, the second line is formed using the formula (10), the third line expresses a longer version of the same integrand in the second line, the fourth line is derived after performing the integration with respect to x_i, where $\partial\mathbb{A}^{\{i\}}$ is the boundary of the domain $\mathbb{A}^{\{i\}}$, and the fifth line is obtained using again the formula (10). Finally, the equality to *zero* in the last line is deduced from the cognizance that at the boundary $\partial\mathbb{A}^{\{i\}}$, the density function is either *zero* or converges to *zero* more rapidly than the rate at which the polynomial $P_{\{i_1,\ldots,i,\ldots,i_{|u|}\},(j_{i_1},\ldots,(j_i-1),\ldots,j_{i_{|u|}})}$ reaches $\pm\infty$ when x_i approaches the boundary. □

Appendix B. Second-moment properties of $y(1;\mathbf{X})$

Applying the expectation operators on (30) and its square, the first two raw moments of $y(1;\mathbf{X})$ are respectively given by (B.1) and (B.2) for the Gaussian density on $\mathbb{R}^3$, by (B.3) and (B.4) for the Gegenbauer density on $\mathbb{B}^3$, and by (B.5) and (B.6) for the Dirichlet density on $\mathbb{T}^3$.

(1) Gaussian density on $\mathbb{R}^3$ ($\sigma_1 = \sigma_2 = \sigma_3 = 1/4$, $\rho_{12} = \rho_{13} = \rho_{23} = 1/5$):

$$
\mathbb{E}\left[y(1;\mathbf{X})\right] = \frac{3441\,\sqrt[32]{e}}{3200} \approx 1.10945. \tag{B.1}
$$

$$
\mathbb{E}\left[y^2(1;\mathbf{X})\right] = \frac{748761\sqrt[8]{e}}{640000} \approx 1.32571. \tag{B.2}
$$

(2) Gegenbauer density on $\mathbb{B}^3$ ($\mu = 5$):

$$\mathbb{E}\left[y(1;\mathbf{X})\right] = 46080\left[I_6(1) + I_7(1)\right] \approx 1.10997. \tag{B.3}$$

$$\mathbb{E}\left[y^2(1;\mathbf{X})\right] = 180\left[7I_6(2) - 17I_7(2)\right] \approx 1.32882. \tag{B.4}$$

(3) Dirichlet density on $\mathbb{T}^3$ ($\kappa_1 = \kappa_2 = \kappa_3 = \kappa_4 = 1$):

$$\mathbb{E}\left[y(1;\mathbf{X})\right] = \frac{32\left[4453I_0\left(\frac{1}{2}\right) - 18321I_1\left(\frac{1}{2}\right)\right]}{231\sqrt{e}} \approx 0.908263. \tag{B.5}$$

$$\mathbb{E}\left[y^2(1;\mathbf{X})\right] = \frac{8\left[10283I_0(1) - 22517I_1(1)\right]}{1001e} \approx 0.862236. \tag{B.6}$$

Here, $I_n(z)$ is a modified Bessel function of the first kind, which satisfies the differential equation: $z^2w'' + zw' - (z^2 + n^2)w = 0$.

References

[1] I. Babuska, F. Nobile, R. Tempone, A stochastic collocation method for elliptic partial differential equations with random input data, SIAM J. Numer. Anal. 45 (3) (2007) 1005–1034.

[2] B. Ganapathysubramanian, N. Zabaras, Sparse grid collocation schemes for stochastic natural convection problems, J. Comput. Phys. (ISSN: 0021-9991) 225 (1) (2007) 652–685, http://dx.doi.org/10.1016/j.jcp.2006.12.014. http://www.sciencedirect.com/science/article/pii/S0021999106006152.

[3] N. Wiener, The homogeneous chaos, Amer. J. Math. 60 (4) (1938) 897–936.

[4] R.H. Cameron, W.T. Martin, The orthogonal development of non-linear functionals in series of fourier-Hermite functionals, Ann. of Math. 48 (1947) 385–392.

[5] S. Smolyak, Quadrature and interpolation formulas for tensor products of certain classes of functions, Dokl. Akad. Nauk SSSR 4 (1963) 240–243.

[6] T. Gerstner, M. Griebel, Numerical integration using sparse grids, Numer. Algorithms 18 (1998) 209–232.

[7] R.E. Caflisch, W. Morokoff, A. Owen, Valuation of mortgage backed securities using brownian bridges to reduce effective dimension, J. Comput. Finance 1 (1997) 27–46.

[8] S. Rahman, A polynomial dimensional decomposition for stochastic computing, Internat. J. Numer. Methods Engrg. 76 (2008) 2091–2116.

[9] S. Rahman, Extended polynomial dimensional decomposition for arbitrary probability distributions, J. Eng. Mech. 135 (12) (2009) 1439–1451.

[10] V. Yadav, S. Rahman, Adaptive-sparse polynomial dimensional decomposition for high-dimensional stochastic computing, Comput. Methods Appl. Mech. Engrg. 274 (2014) 56–83.

[11] S. Rahman, Mathematical properties of polynomial dimensional decomposition, SIAM/ASA J. Uncertain. Quantification 6 (2018) 816–844.

[12] W. Hoeffding, A class of statistics with asymptotically normal distribution, Ann. Math. Stat. (ISSN: 00034851) 19 (3) (1948) pp. 293–325. http://www.jstor.org/stable/2235637.

[13] I.M. Sobol, Sensitivity estimates for nonlinear mathematical models, Math. Model. Comput. Exp. 1 (1993) 407–414.

[14] H. Rabitz, O. Alis, General foundations of high dimensional model representations, J. Math. Chem. (ISSN: 0259-9791) 25 (1999) 197–233 10.1023/A:1019188517934.

[15] S. Rahman, Approximation errors in truncated dimensional decompositions, Math. Comp. 83 (290) (2014) 2799–2819.

[16] M. Griebel, M. Holtz, Dimension-wise integration of high-dimensional functions with applications to finance, J. Complexity 26 (5) (2010) 455–489.

[17] Y. Noh, K.K. Choi, L. Du, Reliability-based design optimization of problems with correlated input variables using a gaussian Copula, Struct. Multidiscip. Optim. 38 (2009) 1–16.

[18] S. Rahman, Dimension-wise multivariate orthogonal polynomials in general probability spaces. arXiv:1810.12113.

[19] C.F. Dunkl, Y. Xu, Orthogonal Polynomials of Several Variables, second ed., in: Encyclopedia of Mathematics and its Applications 155, Cambridge University Press, 2001.

[20] A. Erdélyi, Higher Transcendental Functions, in: Encyclopedia of Mathematics and its Applications 155, vol. II, McGraw-Hill, 1953.

[21] B. Holmquist, The d-variate vector hermite Polynomial of Order k, Linear Algebra Appl. 237/238 (1996) 155–190.

[22] P. Appell, J.K. de Fériet, Fonctions hypergéométriques et hypersphériques, polynomes d'Hermite, 1926, pp. 1–14.

[23] H.L. Krall, I.M. Sheffer, Orthogonal polynomials in two variables, Ann. Mat. Pura Appl. 76 (4) (1967) 325–376.

[24] G.H. Golub, C.F. van Loan, Matrix Computations, third ed., The John Hopkins University Press, 1996.

[25] S. Rahman, Wiener-Hermite polynomial expansion for multivariate Gaussian Probability Measures, J. Appl. Math. Appl. 454 (2017) 303–334.

[26] S. Rahman, A generalized ANOVA Dimensional Decomposition for Dependent Probability Measures, SIAM/ASA J. Uncertain. Quantification 2 (2014) 670–697.

[27] G. Hooker, Generalized functional ANOVA Diagnostics for High-Dimensiobal Functions of Dependent Variables, J. Comput. Graph. Statist. 16 (3) (2007) 709–732.

[28] A. Chakraborty, S. Rahman, Stochastic multiscale models for fracture analysis of functionally graded materials, Eng. Fract. Mech. 75 (2008) 2062–2086.
[29] S. Rahman, V. Yadav, Orthogonal polynomial expansions for solving random eigenvalue problems, Int. J. Uncertain. Quantif. 1 (2) (2011) 163–187.
[30] K. Tang, P.M. Congedo, R. Abgrall, Adaptive surrogate modeling by anova and sparse polynomial dimensional decomposition for global sensitivity analysis in fluid simulation, J. Comput. Phys. 314 (1) (2016) 557–589.
[31] X. Ren, V. Yadav, S. Rahman, Reliability-based design optimization by adaptive-sparse polynomial dimensional decomposition, Struct. Multidiscip. Optim. 53 (3) (2016) 425–452.
[32] S. Rahman, A polynomial chaos expansion in dependent random variables, J. Appl. Math. Appl. 4 (2018) 1–26.
[33] J.K. Cullum, R.A. Willoughby, Lanczos algorithms for large symmetric eigenvalue computations: theory, in: Classics in Applied Mathematics, Society for Industrial and Applied Mathematics, ISBN: 9780898715231, 2002.
[34] H. Niederreiter, Random Number Generation and Quasi-Monte Carlo Methods, in: CBMS-NSF Regional Conference Series in Applied Mathematics, Society for Industrial and Applied Mathematics, ISBN: 9780898712957, 1992. http://books.google.com/books?id=pca2tPZoz XcC.
[35] I.M. Sobol, Distribution of points in a cube and approximate evaluation of integrals, Zh. Vychisl. Mat. Mat. Fiz. 7 (1967) 784–802.
[36] H. Xu, S. Rahman, A generalized dimension-reduction method for multi-dimensional integration in stochastic mechanics, Internat. J. Numer. Methods Engrg. 61 (2004) 1992–2019.