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Global sensitivity analysis by polynomial dimensional decomposition

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ABSTRACT

This paper presents a polynomial dimensional decomposition (PDD) method for global sensitivity analysis of stochastic systems subject to independent random input following arbitrary probability distributions. The method involves Fourier-polynomial expansions of lower-variate component functions of a stochastic response by measure-consistent orthonormal polynomial bases, analytical formulae for calculating the global sensitivity indices in terms of the expansion coefficients, and dimension-reduction integration for estimating the expansion coefficients. Due to identical dimensional structures of PDD and analysis-of-variance decomposition, the proposed method facilitates simple and direct calculation of the global sensitivity indices. Numerical results of the global sensitivity indices computed for smooth systems reveal significantly higher convergence rates of the PDD approximation than those from existing methods, including polynomial chaos expansion, random balance design, state-dependent parameter, improved Sobol's method, and sampling-based methods. However, for non-smooth functions, the convergence properties of the PDD solution deteriorate to a great extent, warranting further improvements. The computational complexity of the PDD method is polynomial, as opposed to exponential, thereby alleviating the curse of dimensionality to some extent.

1. Introduction

Mathematical modeling of complex systems often requires sensitivity analysis to determine how an output variable of interest is influenced by individual or subsets of input variables. A traditional local sensitivity analysis entails gradients or derivatives, often invoked in design optimization, describing changes in the model response due to the local variation of input. Depending on the model output, obtaining gradients or derivatives, if they exist, can be simple or difficult. In contrast, a global sensitivity analysis (GSA), increasingly becoming mainstream, characterizes how the global variation of input, due to its uncertainty, impacts the overall uncertain behavior of the model. In other words, GSA constitutes the study of how the output uncertainty from a mathematical model is divvied up, qualitatively or quantitatively, to distinct sources of input variation in the model [1].

Almost all GSA are based on the second-moment properties of random output, for which there exist a multitude of methods or techniques for calculating the global sensitivity indices. Prominent among them are a random balance design (RBD) method [2], which integrates its previous version [3] with a Fourier amplitude sensitivity test [4]; a state dependent parameter (SDP) meta-model [5] based on recursive filtering and smoothing estimation; and a variant of Sobol's method with an improved formula [6–8]. More recent developments on GSA include application of polynomial chaos expansion (PCE) [9] as a meta-model, commonly used for uncertainty quantification of complex systems [10]. Crestaux et al. [11] examined the PCE method for calculating sensitivity indices by comparing their convergence properties with those from standard sampling-based methods, including Monte Carlo with Latin hypercube sampling (MC-LHS) [12] and quasi-Monte Carlo (QMC) simulation [13]. Their findings reveal faster convergence of the PCE solution relative to sampling-based methods for smoothly varying model responses, but the convergence rate may degrade markedly when confronted with non-smooth systems. They also found the PCE method to be cost effective for low to moderate dimensional systems, even with smooth responses, imposing a heavy computational burden when there exist a mere ten variables or more. Indeed, computational research on GSA is far from complete and, therefore, development of alternative methods for improving the accuracy or efficiency of existing methods is desirable.

This paper presents an alternative method, known as the polynomial dimensional decomposition (PDD) method, for variance-based GSA of stochastic systems subject to independent random input following arbitrary probability distributions. The method is based on (1) Fourier-polynomial expansions of lower-variate component functions of a stochastic response by measure-consistent orthonormal polynomial bases; (2) analytical formulae for calculating the global sensitivity indices in terms of the

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expansion coefficients; and (3) dimension-reduction integration for efficiently estimating the expansion coefficients. Section 2 reviews a generic dimensional decomposition of a multivariate function, including three distinct variants. Section 3 invokes the properties of lower-variate component functions of a dimensional decomposition, leading to a formal definition of the global sensitivity index. The Fourier-polynomial expansion, calculation of sensitivity indices, dimension-reduction integration, including the computational effort, and novelties are described in Section 4. Five numerical examples illustrate the accuracy, convergence properties, and computational efficiency of the proposed method in Section 5. Finally, conclusions are drawn in Section 6.

2. Dimensional decomposition

Let $(\Omega,\mathcal{F},P)$ be a complete probability space, where Ω is a sample space, $\mathcal{F}$ is a σ-field on Ω, and $P:\mathcal{F}\rightarrow[0,1]$ is a probability measure. With $\mathcal{B}^N$ representing the Borel σ-field on $\mathbb{R}^N$, consider an $\mathbb{R}^N$-valued independent random vector $\boldsymbol{X}=\{X_1,\ldots,X_N\}^T:(\Omega,\mathcal{F})\rightarrow(\mathbb{R}^N,\mathcal{B}^N)$, which describes statistical uncertainties in all system and input parameters of a given stochastic problem. The probability law of $\boldsymbol{X}$ is completely defined by the joint probability density function $f_{\boldsymbol{X}}(\boldsymbol{x})=\prod_{i=1}^{i=N}f_i(x_i)$, where $f_i(x_i)$ is the marginal probability density function of X_i defined on the probability triple $(\Omega_i,\mathcal{F}_i,P_i)$. Let $y(\boldsymbol{X}):=y(X_1,\ldots,X_N)$, a real-valued, square-integrable, measurable transformation on $(\Omega,\mathcal{F})$, define a relevant response of the stochastic system. A general dimensional decomposition of $y(\boldsymbol{X})$, described by [14–20]

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

can be viewed as a finite, hierarchical expansion of an output function in terms of its input variables with increasing dimensions, where $\emptyset\neq u\subseteq\{1,\ldots,N\}$ is a subset with the complementary set $-u=\{1,\ldots,N\}-u$ and cardinality $1\leq|u|\leq N$, $y_{\emptyset}$ is a constant, and $y_u(\boldsymbol{X}_u)$ is a $|u|$-variate component function describing the cooperative influence of $\boldsymbol{X}_u$, a subvector of $\boldsymbol{X}$, on y. The summation in Eq. (1) comprises 2^N-1 terms, with each term depending on a group of variables indexed by a particular subset of $\{1,\ldots,N\}$. The origin of dimensional decomposition can be traced to the work of Hoeffding [14] in the 1940s and is well known in the statistics literature as analysis of variance (ANOVA) [15]. This decomposition, later referred to as high-dimensional model representation (HDMR), was subject to further refinements, including cut-HDMR [16] and random-sampling (RS)-HDMR [17]. The author's group examined this decomposition from the perspective of Taylor series expansion, calculating the statistical moments [18,19] and reliability [20] of mechanical systems.

An important feature of the decomposition in Eq. (1) is the selection of the constant $y_{\emptyset}$ and component functions $y_u(\boldsymbol{X}_u)$, $\emptyset\neq u\subseteq\{1,\ldots,N\}$. By defining an error functional associated with a given $y(\boldsymbol{X})$ and an appropriate kernel function, an optimization problem can be formulated and solved to obtain the desired constant and component functions. However, different kernel functions will create distinct yet formally equivalent decompositions, all exhibiting the same structure of Eq. (1). There exist three important variants of the decomposition, described as follows.

2.1. Referential dimensional decomposition

The referential dimensional decomposition (RDD) involves the Dirac measure $\prod_{i=1}^{N}\delta(x_i-c_i)$ at a reference point $\boldsymbol{c}\in\mathbb{R}^N$ as the kernel function, leading to [16,19]

$$y(\boldsymbol{X})=y(\boldsymbol{c})+\sum_{u\subseteq\{1,\ldots,N\}}\sum_{v\subseteq u}(-1)^{|u|-|v|}y(\boldsymbol{X}_v,\boldsymbol{c}_{-v}), \tag{2}$$

where $(\boldsymbol{X}_v,\boldsymbol{c}_{-v})$ denotes an N-dimensional vector whose ith component is X_i if $i\in v$ and c_i if $i\notin v$. Both the recursive form, presented as the cut-HDMR method [16], and the explicit form, in conjunction with the dimension-reduction [19] or decomposition [20] method, of Eq. (2) exist. These two forms, developed independently, have been proved to be equivalent [21]. Nonetheless, the RDD component functions lack orthogonal features, but are easy to obtain as they only involve function evaluations at a chosen reference point.

2.2. ANOVA dimensional decomposition

The ANOVA dimensional decomposition (ADD) entails the probability density function $f_{\boldsymbol{X}}(\boldsymbol{x})$ of $\boldsymbol{X}$ as the kernel function, which results in [15,22]

$$y(\boldsymbol{X})=y_0+\sum_{u\subseteq\{1,\ldots,N\}}\sum_{v\subseteq u}(-1)^{|u|-|v|}\int_{\mathbb{R}^{N-|v|}}y(\boldsymbol{X}_v,\boldsymbol{x}_{-v})f_{\boldsymbol{X}_{-v}}(\boldsymbol{x}_{-v})\,d\boldsymbol{x}_{-v}, \tag{3}$$

where y_0 is an expansion coefficient. Again, there exists a recursive form of Eq. (3) [22]. The ANOVA decomposition also has a few synonyms, notably, Sobol decomposition, which has been used by Sudret [9] and Crestaux et al. [11], among others. While ADD has desirable orthogonal properties, the ANOVA component functions are difficult to obtain, because they require calculation of high-dimensional integrals.

2.3. Polynomial dimensional decomposition

If $\{\psi_{ij}(X_i);j=0,1,\ldots\}$ is a set of orthonormal polynomial basis functions in the Hilbert space $\mathcal{L}_2(\Omega_i,\mathcal{F}_i,P_i)$ and is consistent with the probability measure P_i of X_i, then the ANOVA decomposition can be extended to generate the PDD of [23,24]

$$y(\boldsymbol{X})=y_0+\sum_{u=\{i_1,\ldots,i_{|u|}\}\subseteq\{1,\ldots,N\}}\sum_{j_{i_{|u|}}=1}^{\infty}\cdots\sum_{j_{i_1}=1}^{\infty}C_{i_1\cdots i_{|u|}j_{i_1}\cdots j_{i_{|u|}}}\psi_{i_1j_{i_1}}(X_{i_1})\cdots\psi_{i_{|u|}j_{i_{|u|}}}(X_{i_{|u|}}), \tag{4}$$

where $C_{i_1\cdots i_{|u|}j_{i_1}\cdots j_{i_{|u|}}}$, $1\leq|u|\leq N$, are additional expansion coefficients that also require calculating high-dimensional integrals. The PDD also has orthogonal component functions and exploits the smoothness of y, if any, for efficiently calculating its probabilistic characteristics. The author's recent work reveals that the measure-consistent PDD [24] leads to faster convergence of stochastic solutions, when compared with the traditional ANOVA decomposition employing uniform probability measure, also known as RS-HDMR [17].

3. Global sensitivity analysis

3.1. Variance decomposition

The ADD in Eq. (3) can be written more explicitly as

$$y(\boldsymbol{X})=y_0+\sum_{i=1}^{N}y_i(X_i)+\sum_{i_1=1}^{N-1}\sum_{i_2=i_1+1}^{N}y_{i_1i_2}(X_{i_1},X_{i_2})+\cdots+\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}y_{i_1\cdots i_s}(X_{i_1},\ldots,X_{i_s})+\cdots+y_{12\cdots N}(X_1,\ldots,X_N), \tag{5}$$

where the constant y_0 and component functions $y_{i_1\cdots i_s}(x_{i_1},\ldots,x_{i_s})$, $1\le i_1<\cdots<i_s\le N$, $s=1,\ldots,N$, are obtained from

$$y_0 \coloneqq \int_{\mathbb{R}^N} y(\boldsymbol{x}) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\boldsymbol{x},$$

$$y_i(x_i) \coloneqq \int_{\mathbb{R}^{N-1}} y(\boldsymbol{x}) \prod_{j\neq i} f_j(x_j)\, dx_j - y_0,$$

$$y_{i_1 i_2}(x_{i_1},x_{i_2}) \coloneqq \int_{\mathbb{R}^{N-2}} y(\boldsymbol{x}) \prod_{j\neq [i_1,i_2]} f_j(x_j)\, dx_j - y_{i_1}(x_{i_1}) - y_{i_2}(x_{i_2}) - y_0,$$

$$\vdots$$

$$\begin{aligned} y_{i_1\cdots i_s}(x_{i_1},\ldots,x_{i_s}) \coloneqq \int_{\mathbb{R}^{N-s}} y(\boldsymbol{x}) \prod_{j\neq [i_1,\ldots,i_s]} f_j(x_j)\, dx_j \\ - \sum_{j_1<\cdots<j_{s-1}\subset\{i_1,\ldots,i_s\}} y_{j_1\cdots j_{s-1}}(x_{j_1},\ldots,x_{j_{s-1}}) \\ - \sum_{j_1<\cdots<j_{s-2}\subset\{i_1,\ldots,i_s\}} y_{j_1\cdots j_{s-2}}(x_{j_1},\ldots,x_{j_{s-2}}) \\ - \cdots - \sum_{j\subset\{i_1,\ldots,i_s\}} y_j(x_j) - y_0, \end{aligned} \tag{6}$$

quantifying various main and cooperative effects of input variables on y. If $\mathbb{E}$ is the expectation operator with respect to $f_{\boldsymbol{X}}(\boldsymbol{x})$, then two important properties of the ANOVA decomposition required for uniquely defining its component functions are as follows.

Property 1. *The ANOVA component functions* $y_{i_1\cdots i_s}(X_{i_1},\ldots,X_{i_s})$, $1\le i_1<\cdots<i_s\le N$, $s=1,\ldots,N$, *have zero means, i.e.,*

$$\mathbb{E}[y_{i_1\cdots i_s}(X_{i_1},\ldots,X_{i_s})] \coloneqq \int_{\mathbb{R}^N} y_{i_1\cdots i_s}(x_{i_1},\ldots,x_{i_s}) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\boldsymbol{x} = 0. \tag{7}$$

Property 2. *Two distinct ANOVA component functions* $y_{i_1\cdots i_s}(X_{i_1},\ldots,X_{i_s})$, $1\le i_1<\cdots<i_s\le N$, *and* $y_{j_1\cdots j_t}(X_{j_1},\ldots,X_{j_t})$, $1\le j_i<\cdots<j_t\le N$, *where* $1\le s\le N$, $1\le t\le N$, and $(i_1\ldots i_s)\neq(j_1\ldots j_t)$, *are uncorrelated, i.e., they satisfy the orthogonality property*

$$\begin{aligned} &\mathbb{E}[y_{i_1\cdots i_s}(X_{i_1},\ldots,X_{i_s}) y_{j_1\cdots j_t}(X_{j_1},\ldots,X_{j_t})] \\ &\quad \coloneqq \int_{\mathbb{R}^N} y_{i_1\cdots i_s}(x_{i_1},\ldots,x_{i_s}) y_{j_1\cdots j_t}(x_{j_1},\ldots,x_{j_t}) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\boldsymbol{x} = 0. \end{aligned} \tag{8}$$

Traditionally, Eq. (5) with X_j, $j=1,\ldots,N$, following independent, standard uniform distributions, has been identified as the ANOVA decomposition [15,22]; however, the author's recent work [24] reveals no fundamental requirement for a specific probability measure of $\boldsymbol{X}$, provided that the resultant integrals in Eq. (6) exist and are finite.

Applying the expectation operator on $y(\boldsymbol{X})$ in Eq. (5) and noting Property 1, the mean $\mathbb{E}[y(\boldsymbol{X})]=y_0$, the first coefficient of ADD appearing in the first line of Eq. (6). Applying the expectation operator again, this time on $(y(\boldsymbol{X})-y_0)^2$, and recognizing Property 2 results in splitting the variance

$$\begin{aligned} \sigma^2 &\coloneqq \mathbb{E}[(y(\boldsymbol{X})-y_0)^2] = \sum_{i=1}^{N} \sigma_i^2 + \sum_{i_1=1}^{N-1}\sum_{i_2=i_1+1}^{N} \sigma_{i_1 i_2}^2 + \cdots \\ &\quad + \sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N} \sigma_{i_1\cdots i_s}^2 + \cdots + \sigma_{12\cdots N}^2 \\ &= \sum_{s=1}^{N} \left(\underbrace{\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}}_{s \text{ sums}} \sigma_{i_1\cdots i_s}^2 \right) \end{aligned} \tag{9}$$

of $y(\boldsymbol{X})$, where the variance contribution

$$\sigma_{i_1\cdots i_s}^2 \coloneqq \mathbb{E}[y_{i_1\cdots i_s}^2(X_{i_1},\ldots,X_{i_s})] \coloneqq \int_{\mathbb{R}^N} y_{i_1\cdots i_s}^2(x_{i_1},\ldots,x_{i_s}) f_{\boldsymbol{X}}(\boldsymbol{x})\, d\boldsymbol{x} \tag{10}$$

to the total sum comes from the corresponding *zero*-mean s-variate component function. According to Eq. (9), the variance decomposition follows the same structure of $y(\boldsymbol{X})-y_0$ from Eq. (5), explaining why the acronym "ANOVA" is also coined for the function decomposition.

3.2. Global sensitivity index

The s-variate global sensitivity index[1] of a stochastic response function $y(\boldsymbol{X})$ for a set $\{X_{i_1},\ldots,X_{i_s}\}$ of input variables, denoted by $S_{\{i_1,\ldots,i_s\}}$, is defined as the non-negative ratio [6]

$$S_{\{i_1,\ldots,i_s\}} \coloneqq \frac{\sigma_{i_1\cdots i_s}^2}{\sigma^2}, \quad \sigma>0, \tag{11}$$

representing the fraction of the variance of $y(\boldsymbol{X})$ contributed by $y_{i_1\cdots i_s}(X_{i_1},\ldots,X_{i_s})$. Since $1\le i_1<\cdots<i_s\le N$ and $s=1,\ldots,N$, there exist 2^N-1 such indices, adding up to

$$\sum_{s=1}^{N} \left(\underbrace{\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}}_{s \text{ sums}} S_{\{i_1,\ldots,i_s\}} \right) = 1. \tag{12}$$

For example, when $N=3$, there are seven global sensitivity indices: three univariate indices ($S_{\{1\}},S_{\{2\}},S_{\{3\}}$) due to the main effects, three bivariate indices ($S_{\{1,2\}},S_{\{1,3\}},S_{\{2,3\}}$) due to the cooperative effects of two variables, and a trivariate index ($S_{\{1,2,3\}}$) due to the cooperative effect of three variables.

The global sensitivity indices illuminate the dimensional structure lurking behind a complex response function. The indices can be used to rank variables, fix unessential variables, and reduce dimensions of large-scale problems [25]. In many applications, the response function y with a low effective dimension [26] can be approximated by combinations of low-variate component functions, requiring, consequently, only low-variate sensitivity indices. For instance, if $y(\boldsymbol{X}) = y_0 + \sum_{i=1}^{i=N} y_i(X_i) + \sum_{i_1=1}^{N-1}\sum_{i_2=i_1+1}^{N} y_{i_1 i_2}(X_{i_1},X_{i_2})$ represents an N-variate function comprising at most bivariate component functions, then only the univariate and bivariate sensitivities need to be determined and all higher-variate sensitivities are equal to *zero*, satisfying $\sum_{i=1}^{N} S_{\{i\}} + \sum_{i_1=1}^{N-1}\sum_{i_2=i_1+1}^{N} S_{\{i_1,i_2\}} = 1$. However, a naive or direct calculation of sensitivity indices, low-variate or not, would require integral evaluations of the constant and component functions in Eq. (5), followed by numerous integral evaluations of sensitivity indices desired. For high-dimensional systems, such an approach is impractical and possibly prohibitive. Therefore, alternative routes must be charted to estimate the sensitivity indices both accurately and efficiently.

4. Polynomial dimensional decomposition method

4.1. Fourier-polynomial expansion

Defined on the product probability triple $\left(\times_{p=1}^{p=s}\Omega_{i_p}, \times_{p=1}^{p=s}\mathcal{F}_{i_p}, \times_{p=1}^{p=s}P_{i_p}\right)$, $1\le s\le N$, denote the space of square integrable s-variate component functions of y by

$$\begin{aligned} \mathcal{L}_2\left(\times_{p=1}^{p=s}\Omega_{i_p}, \times_{p=1}^{p=s}\mathcal{F}_{i_p}, \times_{p=1}^{p=s}P_{i_p}\right) \coloneqq \Big\{ y_{i_1\cdots i_s}(X_{i_1},\ldots,X_{i_s}) : \int_{\mathbb{R}^s} y_{i_1\cdots i_s}^2(x_{i_1},\ldots,x_{i_s}) \\ \times \prod_{p=1}^{s} f_{i_p}(x_{i_p})\, dx_{i_p} < \infty \Big\}, \end{aligned} \tag{13}$$

[1] Since an s-variate component function may contain arbitrarily high-order (*i.e.*, higher than s-order) terms, depending on the nonlinearity of the response, the appellation of the term "s-variate global sensitivity index" is more appropriate than the term "s-order global sensitivity index".

which is a Hilbert space. Since the joint density of $\{X_{i_1},\ldots,X_{i_s}\}^T$ is separable (independence), the tensor product $\prod_{p=1}^{s}\psi_{i_pj_p}(X_{i_p}) = \psi_{i_1j_1}(X_{i_1})\cdots\psi_{i_sj_s}(X_{i_s})$ constitutes an orthonormal polynomial basis in $\mathcal{L}_2$. Therefore, there exists a Fourier-polynomial expansion of

$$y_{i_1\cdots i_s}(X_{i_1},\ldots,X_{i_s}) = \sum_{j_s=1}^{\infty}\cdots\sum_{j_1=1}^{\infty} C_{i_1\cdots i_sj_1\cdots j_s}\prod_{p=1}^{s}\psi_{i_pj_p}(X_{i_p}) \tag{14}$$

involving

$$C_{i_1\cdots i_sj_1\cdots j_s} \coloneqq \int_{\mathbb{R}^N} y(\boldsymbol{x})\prod_{p=1}^{s}\psi_{i_pj_p}(x_{i_p}) f_{\boldsymbol{X}}(\boldsymbol{x})\,d\boldsymbol{x} \tag{15}$$

as the generic s-variate expansion coefficient. Applying the expansion in Eq. (14) into Eq. (5) for $1\le i_1<\cdots<i_s\le N$ and $s=1,\ldots,N$ yields

$$y(\boldsymbol{X}) = y_0 + \sum_{s=1}^{N}\left[\underbrace{\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}}_{s\text{ sums}}\underbrace{\sum_{j_1=1}^{\infty}\cdots\sum_{j_s=1}^{\infty}}_{s\text{ sums}} C_{i_1\cdots i_sj_1\cdots j_s}\prod_{p=1}^{s}\psi_{i_pj_p}(X_{i_p})\right], \tag{16}$$

an explicit form of Eq. (4). Once the embedded coefficients are calculated, as described in a forthcoming subsection, Eq. (16) furnishes an explicit map $y:\mathbb{R}^N\to\mathbb{R}$, describing an input–output relationship from a complex numerical analysis or algorithm. Consequently, GSA or second-moment analysis of $y(\boldsymbol{X})$ can be easily conducted using Eq. (16).

4.2. Calculation of global sensitivity indices

For calculating $\sigma^2_{i_1\cdots i_s}$ and σ^2 using orthonormal polynomials, two important properties of $\psi_{ij}(X_i)$ are required and are described as follows.

Property 3. *The orthonormal polynomial basis functions have a unit mean for $j=0$ and zero means for all $j\ge 1$, i.e.,*

$$\mathbb{E}[\psi_{ij}(X_i)] \coloneqq \int_{\mathbb{R}}\psi_{ij}(x_i)f_i(x_i)\,dx_i = \begin{cases}1 & \text{if } j=0,\\ 0 & \text{if } j\ge 1.\end{cases} \tag{17}$$

Property 4. *Any two orthonormal polynomial basis functions $\psi_{ij_1}(X_i)$ and $\psi_{ij_2}(X_i)$, where $j_1,j_2=0,1,2,\ldots$, are uncorrelated and each has unit variance, i.e.,*

$$\mathbb{E}[\psi_{ij_1}(X_i)\psi_{ij_2}(X_i)] \coloneqq \int_{\mathbb{R}}\psi_{ij_1}(x_i)\psi_{ij_2}(x_i)f_i(x_i)\,dx_i = \begin{cases}1 & \text{if } j_1=j_2,\\ 0 & \text{if } j_1\ne j_2.\end{cases} \tag{18}$$

Properties 3 and 4 of PDD ensure fulfillment of Properties 1 and 2 of ADD. Readers interested in further explanation of these properties, including details of orthogonal polynomials for an arbitrary probability measure, are referred to the author's prior work [27].

Applying the expectation operator on Eq. (16) and noting Property 3, the mean $\mathbb{E}[y(\boldsymbol{X})]=y_0$ from PDD matches the mean from ADD. Applying the expectation operator on $[y(\boldsymbol{X})-y_0]^2$ yields

$$\sigma^2 = \sum_{s=1}^{N}\sum_{t=1}^{N}\left(\underbrace{\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}\sum_{j_1=1}^{\infty}\cdots\sum_{j_s=1}^{\infty}}_{2s\text{ sums}}\right.$$

$$\left.\times\underbrace{\sum_{k_1=1}^{N-t+1}\cdots\sum_{k_t=k_{t-1}+1}^{N}\sum_{l_1=1}^{\infty}\cdots\sum_{l_t=1}^{\infty}}_{2t\text{ sums}} C_{i_1\cdots i_sj_1\cdots j_s}\times C_{k_1\cdots k_tl_1\cdots l_t}\mathbb{E}\left[\prod_{p=1}^{s}\psi_{i_pj_p}(X_{i_p})\prod_{p=1}^{t}\psi_{k_pl_p}(X_{k_p})\right]\right). \tag{19}$$

The number of summations inside the parenthesis of the right side of Eq. (19) is $2(s+t)$, where s and t are the indices of the two outer summations. By virtue of Property 4 and independent coordinates of $\boldsymbol{X}$,

$$\mathbb{E}\left[\prod_{p=1}^{s}\psi_{i_pj_p}(X_{i_p})\prod_{p=1}^{t}\psi_{k_pl_p}(X_{k_p})\right] = \prod_{p=1}^{s}\mathbb{E}[\psi^2_{i_pj_p}(X_{i_p})] = 1 \tag{20}$$

for $s=t$, $i_p=k_p$, $j_p=l_p$ and *zero* otherwise, leading to

$$\sigma^2 = \sum_{s=1}^{N}\left(\underbrace{\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}}_{s\text{ sums}}\underbrace{\sum_{j_1=1}^{\infty}\cdots\sum_{j_s=1}^{\infty}}_{s\text{ sums}} C^2_{i_1\cdots i_sj_1\cdots j_s}\right) \tag{21}$$

as the sum of squares of the expansion coefficients from PDD of $y(\boldsymbol{X})$. Similarly, applying the expectation operator on $y^2_{i_1\cdots i_s}(X_{i_1},\ldots,X_{i_s})$ from Eq. (14) and invoking Property 4 results in

$$\sigma^2_{i_1\cdots i_s} = \underbrace{\sum_{j_1=1}^{\infty}\cdots\sum_{j_s=1}^{\infty}}_{s\text{ sums}} C^2_{i_1\cdots i_sj_1\cdots j_s}. \tag{22}$$

Therefore, the global sensitivity index $S_{\{i_1,\ldots,i_s\}}$, defined in Eq. (11), can be expressed by

$$S_{\{i_1,\ldots,i_s\}} = \frac{\sum_{j_1=1}^{\infty}\cdots\sum_{j_s=1}^{\infty} C^2_{i_1\cdots i_sj_1\cdots j_s}}{\sum_{s=1}^{N}\left(\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}\sum_{j_1=1}^{\infty}\cdots\sum_{j_s=1}^{\infty} C^2_{i_1\cdots i_sj_1\cdots j_s}\right)} \tag{23}$$

in terms of the expansion coefficients.

Although Eq. (23) provides an exact formula for calculating the global sensitivity index, its numerator and denominator both contain an infinite number of coefficients, emanating from infinite orthonormal polynomials in the PDD of $y(\boldsymbol{X})$ (Eq. (16)). In practice, the number of coefficients must be finite, say, by retaining $1\le m<\infty$ coefficients or polynomials in each variable. Furthermore, in many applications, the function y in Eq. (16) can be approximated by a sum of at most S-variate component functions, where $1\le S\le N$ is the truncation parameter, resulting in the S-variate approximation

$$\tilde{y}_S(\boldsymbol{X}) = y_0 + \sum_{s=1}^{S}\left[\underbrace{\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}}_{s\text{ sums}}\underbrace{\sum_{j_1=1}^{m}\cdots\sum_{j_s=1}^{m}}_{s\text{ sums}} C_{i_1\cdots i_sj_1\cdots j_s}\prod_{p=1}^{s}\psi_{i_pj_p}(X_{i_p})\right], \tag{24}$$

which converges to $y(\boldsymbol{X})$ in the mean square sense when $S\to N$ and $m\to\infty$. As a result, the approximate variance $\tilde{\sigma}^2_S$ and approximate variance component $\tilde{\sigma}^2_{i_1\cdots i_s}$ due to the truncated PDD and/or finite number of orthonormal polynomials are

$$\tilde{\sigma}^2_S = \sum_{s=1}^{S}\left(\underbrace{\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}}_{s\text{ sums}}\underbrace{\sum_{j_1=1}^{m}\cdots\sum_{j_s=1}^{m}}_{s\text{ sums}} C^2_{i_1\cdots i_sj_1\cdots j_s}\right) \tag{25}$$

and

$$\tilde{\sigma}^2_{i_1\cdots i_s} = \underbrace{\sum_{j_1=1}^{m}\cdots\sum_{j_s=1}^{m}}_{s\text{ sums}} C^2_{i_1\cdots i_sj_1\cdots j_s},\quad s=1,\ldots,S, \tag{26}$$

respectively, leading to the approximate global sensitivity index

$$\tilde{S}_{\{i_1,\ldots,i_s\}} \coloneqq \frac{\tilde{\sigma}^2_{i_1\cdots i_s}}{\tilde{\sigma}^2_S} = \frac{\sum_{j_1=1}^{m}\cdots\sum_{j_s=1}^{m} C^2_{i_1\cdots i_s j_1\cdots j_s}}{\sum_{s=1}^{S}\left(\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}\sum_{j_1=1}^{m}\cdots\sum_{j_s=1}^{m} C^2_{i_1\cdots i_s j_1\cdots j_s}\right)} \tag{27}$$

of $y(\boldsymbol{X})$ for any $s=1,\ldots,S$ and satisfying

$$\sum_{s=1}^{S}\left(\underbrace{\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}}_{s\text{ sums}}\tilde{S}_{\{i_1,\ldots,i_s\}}\right)=1. \tag{28}$$

Note that $\tilde{S}_{\{i_1,\ldots,i_s\}}$ for a given set $\{X_{i_1},\ldots,X_{i_s}\}$ of input variables depends on S and m, and should converge to $S_{\{i_1,\ldots,i_s\}}$ as $S\to N$ and $m\to\infty$. However, its convergence with respect to m can be quite complicated, depending mostly on the smoothness property of y. The PCE method also exploits the smoothness condition by including the same orthogonal polynomials, leading to similar equations for sensitivity indices [11], but it lacks the dimensional hierarchy of PDD exhibited in Eqs. (16) or (24). For GSA of a given stochastic system, it will be intriguing to find if, indeed, PDD is superior to PCE or *vice versa*.

For statistically dependent random variables, PDD requires constructing multivariate orthogonal polynomials for a general, multivariate joint density function. New methods avoiding nonlinear transformations will need to be developed for generating measure-consistent multivariate polynomials. Stochastic problems entailing dependent random variables are outside the scope of the present work.

4.3. Dimension-reduction integration for calculating expansion coefficients

The determination of the expansion coefficients, which involve N-dimensional integrals over $\mathbb{R}^N$, is computationally prohibitive when N is large. Instead, a dimension-reduction integration, presented as follows, was applied to estimate the coefficients efficiently.

Let $\boldsymbol{c}=\{c_1,\ldots,c_N\}^T$ be a reference point of input $\boldsymbol{X}$ and $y(c_1,\ldots,c_{i_1-1},X_{i_1},c_{i_1+1},\ldots,c_{i_{R-k}-1},X_{i_{R-k}},c_{i_{R-k}+1},\ldots,c_N)$ represent an $(R-k)$th dimensional component function of $y(\boldsymbol{X})$, where $1\le R<N$ is an integer, $k=0,\ldots,R$, and $1\le i_1<\cdots<i_{R-k}\le N$. For example, when $R=1$, the zero-dimensional component function, which is a constant, is $y(\boldsymbol{c})$ and the one-dimensional component functions are $y(X_1,c_2,\ldots,c_N)$, $y(c_1,X_2,\ldots,c_N),\ldots,y(c_1,c_2,\ldots,X_N)$. Using Xu and Rahman's multivariate function theorem [19], it can be shown that the R-variate RDD approximation of $y(\boldsymbol{X})$, defined by

$$\hat{y}_R(\boldsymbol{X}) \coloneqq \sum_{k=0}^{R}(-1)^k\binom{N-R+k-1}{k}\times\underbrace{\sum_{i_1=1}^{N-R+k+1}\cdots\sum_{i_{R-k}=i_{R-k-1}+1}^{N}}_{(R-k)\text{sums}} \times y(c_1,\ldots,c_{i_1-1},X_{i_1},c_{i_1+1},\ldots,c_{i_{R-k}-1},X_{i_{R-k}},c_{i_{R-k}+1},\ldots,c_N), \tag{29}$$

consists of all terms of the Taylor series of $y(\boldsymbol{X})$ that have less than or equal to R variables. The expanded form of Eq. (29), when compared with the Taylor expansion of $y(\boldsymbol{X})$, indicates that the residual error in $\hat{y}_R(\boldsymbol{X})$ includes terms of dimensions $R+1$ and higher. All higher-order R- and lower-variate terms of $y(\boldsymbol{X})$ are included in Eq. (29), which should therefore generally provide a higher-order approximation of a multivariate function than equations derived from first- or second-order Taylor expansions. Therefore, for $R<N$, an N-dimensional integral can be efficiently estimated by at most R-dimensional integrations, if the contributions from terms of dimensions $R+1$ and higher are negligible.

Substituting $y(\boldsymbol{x})$ in Eqs. (6) (first line) and (15) by $\hat{y}_R(\boldsymbol{x})$, the coefficients can be estimated from

$$y_0 \cong \sum_{k=0}^{R}(-1)^k\binom{N-R+k-1}{k}\underbrace{\sum_{i_1=1}^{N-R+k+1}\cdots\sum_{i_{R-k}=i_{R-k-1}+1}^{N}}_{(R-k)\text{sums}} \times\int_{\mathbb{R}^{R-k}} y(c_1,\ldots,c_{i_1-1},x_{i_1},c_{i_1+1},\ldots,c_{i_{R-k}-1},x_{i_{R-k}},c_{i_{R-k}+1},\ldots,c_N) \times\prod_{q=1}^{R-k} f_{k_q}(x_{k_q})\,dx_{k_q} \tag{30}$$

and

$$C_{i_1\cdots i_s j_1\cdots j_s} \cong \sum_{k=0}^{R}(-1)^k\binom{N-R+k-1}{k}\underbrace{\sum_{i_1=1}^{N-R+k+1}\cdots\sum_{i_{R-k}=i_{R-k-1}+1}^{N}}_{(R-k)\text{sums}} \times\int_{\mathbb{R}^{R-k}} y(c_1,\ldots,c_{i_1-1},x_{i_1},c_{i_1+1},\ldots,c_{i_{R-k}-1},x_{i_{R-k}},c_{i_{R-k}+1},\ldots,c_N) \times\prod_{p=1}^{s}\psi_{i_p j_p}(x_{i_p})\prod_{q=1}^{R-k} f_{k_q}(x_{k_q})\,dx_{k_q}, \tag{31}$$

which require evaluating at most R-dimensional integrals. Eqs. (30) and (31), which facilitate calculation of coefficients approaching their exact values as $R\to N$, are more efficient than performing one N-dimensional integration, as in Eqs. (6) and (15), particularly when $R\ll N$. Hence, the computational effort in calculating the coefficients is significantly lowered using the dimension-reduction integration. When $R=1$, 2, or 3, Eqs. (30) and (31) involve one-, at most two-, and at most three-dimensional integrations, respectively. Nonetheless, numerical integration is still required for a general function y. The integration points and associated weights depend on the probability distribution of X_i, and are readily available for classical distribution functions, *e.g.*, the Gauss–Hermite quadrature rule when X_i follows Gaussian distribution [28]. For an arbitrary probability distribution of X_i, the Stieltjes procedure can be employed to generate the appropriate Gauss quadrature formulae [24]. In performing the dimension-reduction integration, the value of R should be selected in such a way that it is either equal to or greater than the value of s. Then the expansion coefficient $C_{i_1\cdots i_s j_1\cdots j_s}$ will have non-trivial solutions.

4.4. Computational effort

The S-variate approximation of the PDD method requires evaluation of the deterministic coefficients: y_0 and $C_{i_1\cdots i_s j_1\cdots j_s}$, $s=1,\ldots,S$, $1\le i_1<\cdots<i_s\le N$, $j_1,\ldots j_s=1,\ldots,m$. If these coefficients are estimated by dimension-reduction integration with $R=S<N$ and, therefore, involve at most S-dimensional tensor product of an n-point univariate quadrature rule depending on m in Eqs. (30) and (31), then the following deterministic responses (function evaluations) are required: $y(\boldsymbol{c})$, $y(c_1,\ldots,c_{i_1-1},x^{(k_1)}_{i_1},c_{i_1+1},\ldots,c_{i_s-1},x^{(k_s)}_{i_s},c_{i_s+1},\ldots,c_N)$ for $k_1,\ldots,k_s=1,\ldots,n(m)$, where the superscripts on variables indicate corresponding integration points. Therefore, the total cost for the S-variate PDD approximation entails a maximum of $\sum_{k=0}^{k=S}\binom{N}{S-k}n^{S-k}(m)$ function evaluations. If the integration points include a common point in each coordinate – a special case of symmetric input probability density functions and odd values of n (see Examples 2, 3 ($N=8$), and 4) – the number of function evaluations reduces to $\sum_{k=0}^{k=S}\binom{N}{S-k}(n(m)-1)^{S-k}$. For instance, the univariate ($S=R=1$), bivariate ($S=R=2$), and trivariate ($S=R=3$) approximations require $(n-1)N+1$ (linear), $N(N-1)(n-1)^2/2+(n-1)N+1$ (quadratic), and $N(N-1)(N-2)(n-1)^3/6+N(N-1)(n-1)^2/2+(n-1)N+1$ (cubic) function evaluations, respectively. In other words, the computational

complexity of the S-variate PDD approximation is Sth-order polynomial, as opposed to exponential, with respect to the number of random variables or integration points. Therefore, PDD ameliorates the curse of dimensionality to some extent.

A recent work by the author's group developed an alternative form of PCE, where the pth-order PCE approximation can be expressed in terms of the PDD coefficients directly [29]. The coefficients can again be estimated by dimension-reduction integration by selecting $R=p<N$, and therefore involving at most p-dimensional tensor product of an n-point univariate quadrature rule, where n depends on p. As a result, the total cost for the pth-order PCE approximation consists of a maximum of $\sum_{k=0}^{k=p}\binom{N}{p-k}n^{p-k}(p)$ function evaluations. The significance of this finding is that the ratio, $\sum_{k=0}^{k=p}\binom{N}{p-k}n^{p-k}(p)/\sum_{k=0}^{k=S}\binom{N}{S-k}n^{S-k}(m)$, can be used to compare the computational efforts by PCE and PDD for identical expansion orders ($m=p$). For example, Figs. 1(a) and (b) present plots of the ratio of numbers of function evaluations by the PCE and PDD approximations as a function of the dimension N for two cases of identical expansion orders: $m=p=3$ and $m=p=5$, respectively, where $n=m+1=p+1$. The plots in each figure were developed separately for $S=1$ (univariate), $S=2$ (bivariate), and $S=3$ (trivariate) PDD approximations. From the results of Figs. 1(a) and (b), regardless of the plot, the ratios are mostly larger than one, indicating greater computational need by the PCE approximation than by the PDD approximation. When $S\ll N$ and $m=p\gg 1$, the PCE approximation is significantly more expensive than the PDD approximation.

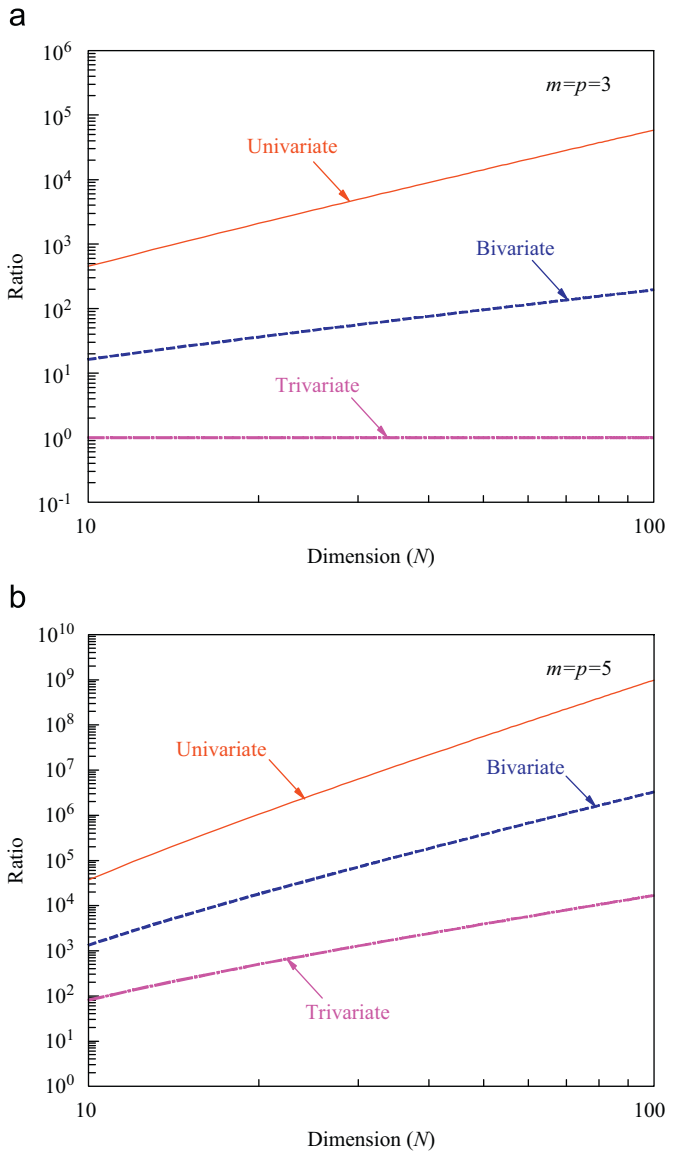

Fig. 1. Ratio of function evaluations by the PCE and PDD approximations for two identical polynomial expansion orders: (a) $m=p=3$ and (b) $m=p=5$. Note: a ratio greater than one indicates higher computational cost of the PCE approximation than the PDD approximation.

4.5. Novelties

Many researchers, including a few cited in this paper [1,2,5–8], readily exploit the RDD (cut-HDMR) or ANOVA decomposition for GSA, including an application for learning the topology of a functional network [30]. However, the ANOVA decomposition in its standard form requires independent random variables that are uniformly distributed over the unit hypercube $[0,1]^N$. When input random variables are independent, but otherwise follow arbitrary probability distributions – a more general case addressed here – one must transform all original random variables into uniform random variables, so that a probabilistic response function can be expanded in terms of classical polynomials. Unfortunately, recent works have shown such transformations to be deleterious, as they may induce overly large nonlinearity of a stochastic response, potentially degrading the convergence properties of probabilistic solutions [24]. The PDD method developed here sidesteps this dicey issue by employing non-classical orthogonal polynomials that are consistent with the probability measure of the random input. By exploiting its orthogonal structure, the method proposes new explicit formulae for the overall variance and its components of a stochastic response in terms of the expansion coefficients. In addition, the method includes a novel dimension-reduction technique that is required for estimating the expansion coefficients efficiently. They constitute a significant departure from existing ANOVA-based methods or techniques employed by others. Finally, it is important to emphasize that this paper exploits for the very first time the PDD approximation of a stochastic response for GSA.

5. Numerical examples

Five numerical examples involving four well-known mathematical functions from the literature and an industrial-scale solid-mechanics problem are presented to illustrate the proposed PDD method for calculating the global sensitivity indices. The mathematical functions selected are smooth or non-smooth, permit exact solutions of the sensitivity indices, and have been studied using a number of existing methods, facilitating a critical evaluation of the PDD method developed. Whenever possible, the classical orthogonal polynomials and associated Gauss quadrature formulae were employed to evaluate the expansion coefficients. The expansion coefficients in Examples 1 and 3 ($N=3$) were calculated by full N-dimensional integrations. However, in Examples 2, 3 ($N=8$), 4, and 5, the coefficients were estimated by dimension-reduction integration with the mean input as the reference point and $R=S$, so that an S-variate PDD approximation requires at most S-variate numerical integration.

For determining the accuracy of the PDD method, three types of error measures were defined: (1) $\mathcal{L}_1$-error in calculating all 2^N-1 sensitivity indices, *i.e.*,

$$e_1 := \sum_{s=1}^{N}\left(\underbrace{\sum_{i_1=1}^{N-s+1}\cdots\sum_{i_s=i_{s-1}+1}^{N}}_{s\text{ sums}}|S_{\{i_1,\ldots,i_s\}}-\tilde{S}_{\{i_1,\ldots,i_s\}}|\right), \tag{32}$$

(2) $\mathcal{L}_1$-error in calculating N univariate sensitivity indices, *i.e.*,

$$e_2 := \sum_{i=1}^{N} |S_{\{i\}} - \tilde{S}_{\{i\}}|, \tag{33}$$

and (3) relative error in calculating each non-zero univariate sensitivity index, *i.e.*,

$$e_{3,i} := \frac{|S_{\{i\}} - \tilde{S}_{\{i\}}|}{S_{\{i\}}}, \quad S_{\{i\}} > 0, \quad i = 1, \ldots, N, \tag{34}$$

where $S_{\{i_1,\ldots,i_s\}}$ is the exact s-variate sensitivity index and $\tilde{S}_{\{i_1,\ldots,i_s\}}$ is the approximate s-variate sensitivity index computed by the S-variate PDD method. Similar error measures from several existing methods were also analyzed and compared with those from the PDD method when appropriate.

5.1. Example 1: polynomial function

Consider the polynomial function

$$y(\boldsymbol{X}) = \frac{1}{2^N} \prod_{i=1}^{N} (3X_i^2 + 1) \tag{35}$$

studied by Sudret [9], where X_i, $i = 1, \ldots N$, are independent and identical random variables, each following standard uniform distribution over [0,1]. From elementary calculations, the exact mean $\mathbb{E}[y(\boldsymbol{X})] = 1$, the variance $\sigma^2 = (6/5)^N - 1$, and the sensitivity indices $S_{\{i_1,\ldots,i_s\}} = 5^{-s}/[(6/5)^N - 1]$, $1 \le i_1 < \cdots < i_s \le N$, $s = 1, \ldots, N$.

For $N=3$, examined here, Eq. (35) represents a sixth-order, trivariate, polynomial function, which is a product of three quadratic polynomials in each variable. Therefore, a trivariate PDD approximation ($S=3$) with second-order ($m=2$) Legendre polynomials (interval$=[-1,+1]$) in Eq. (24) should exactly reproduce y. Since X_1, X_2, and X_3 are independent, the highest order of integrands for calculating the expansion coefficients is four. A three-point Gauss–Legendre quadrature should then provide the exact values of all coefficients. Therefore, if the expansion coefficients are calculated using $m \ge 2$ in Eq. (24) and Eqs. (6) (first line) and (15) are numerically integrated with $n \ge m+1$, then the only source of error in a truncated PDD is the selection of S.

Table 1 presents the estimated global sensitivity indices $\tilde{S}_{\{i_1,\ldots,i_s\}}$, $1 \le i_1 < \cdots < i_s \le S$, $s = 1, \ldots, S$, by univariate ($S=1$), bivariate ($S=2$), and trivariate ($S=3$) PDD approximations, which were calculated separately using $m=1$, $n=2$ and $m=2$, $n=3$, involving only 8 and 27 function evaluations, respectively. Since y is a trivariate function, only the trivariate PDD approximation provides all sensitivity indices. In contrast, the univariate or bivariate PDD approximation yields univariate or at most bivariate sensitivity indices, regardless of m or n. Nonetheless, the predicted indices from all three variants of PDD are reasonably close to each other. When $m=2$, $n=3$, all seven indices generated by the trivariate PDD approximation coincide with the exact indices $S_{\{i_1,\ldots,i_s\}}$, also listed in Table 1, as expected. Sudret solved the same problem using the PCE approximation with the expansion order (p) varying from three to six and correspondingly requiring 29 to 116 function evaluations. The sensitivity indices by the PCE approximation enumerated in Table 1 also converge to the exact solutions when $p=6$, an order three times larger than the order of univariate polynomials required by the PDD method. At exactness, PDD is more efficient than PCE by a factor of $116/27 \cong 4.3$. The higher efficiency of the PDD method is attributed to its dimensional hierarchy, favorably exploiting the structure of y.

5.2. Example 2: non-polynomial function

The second example involves GSA of the Ishigami and Homma function [31]

$$y(\boldsymbol{X}) = \sin X_1 + a\sin^2 X_2 + bX_3^4 \sin X_1, \tag{36}$$

where X_i, $i=1,2,3$, are three independent and identically distributed uniform random variables on $[-\pi, +\pi]$, and a and b are real-valued deterministic parameters. This function, studied by several researchers [9,11], also permits exact solutions of the variance and sensitivity indices as follows: variance $\sigma^2 = a^2/8 + b\pi^4/5 + b^2\pi^8/18 + 1/2$, sensitivity indices $S_{\{1\}} = [b\pi^4/5 + b^2\pi^8/50 + 1/2]/\sigma^2$, $S_{\{2\}} = [a^2/8]/\sigma^2$, $S_{\{3\}} = 0$, $S_{\{1,2\}} = 0$, $S_{\{1,3\}} = [8b^2\pi^8/225]/\sigma^2$, $S_{\{2,3\}} = 0$, and $S_{\{1,2,3\}} = 0$. Note that y is a non-polynomial function; therefore, neither PDD nor PCE will provide exact solutions, but their respective errors can be reduced to an arbitrarily low value by increasing the polynomial orders successively. In this example, the following deterministic parameters were selected: $a=7$, $b=0.1$.

Since the right hand side of Eq. (36) includes cooperative effects of at most two variables, the bivariate PDD approximation is adequate for convergence analysis. In this example, the expansion coefficients of the bivariate approximation were estimated using Legendre polynomials (interval$=[-1,+1]$) of specified order m and dimension-reduction integration (Gauss–Legendre quadrature rule) with $R=S=2$. Since the integrand is not polynomial, the optimal value of n for a specified m is difficult to

Table 1
Approximate and exact sensitivity indices of the polynomial function by various methods (Example 1).

Sensitivity index & L	Univariate PDD ($S=1$)[a]		Bivariate PDD ($S=2$)[a]		Trivariate PDD ($S=3$)[a]		PCE[b]				Exact[c,d]
	$m=1$	$m=2$	$m=1$	$m=2$	$m=1$	$m=2$[c]	$p=3$	$p=4$	$p=5$	$p=6$[c]	
$\tilde{S}_{\{1\}}, S_{\{1\}}$	0.3333	0.3333	0.2807	0.2778	0.2780	0.2747	0.2879	0.2725	0.2747	0.2747	0.2747
$\tilde{S}_{\{2\}}, S_{\{2\}}$	0.3333	0.3333	0.2807	0.2778	0.2780	0.2747	0.2773	0.2733	0.2747	0.2747	0.2747
$\tilde{S}_{\{3\}}, S_{\{3\}}$	0.3333	0.3333	0.2807	0.2778	0.2780	0.2747	0.2773	0.2737	0.2747	0.2747	0.2747
$\tilde{S}_{\{1,2\}}, S_{\{1,2\}}$	–	–	0.0526	0.0556	0.0521	0.0549	0.0506	0.0564	0.0550	0.0549	0.0549
$\tilde{S}_{\{1,3\}}, S_{\{1,3\}}$	–	–	0.0526	0.0556	0.0521	0.0549	0.0506	0.0564	0.0550	0.0549	0.0549
$\tilde{S}_{\{2,3\}}, S_{\{2,3\}}$	–	–	0.0526	0.0556	0.0521	0.0549	0.0481	0.0569	0.0550	0.0549	0.0549
$\tilde{S}_{\{1,2,3\}}, S_{\{1,2,3\}}$	–	–	–	–	0.0098	0.0110	0.0081	0.0108	0.0110	0.0110	0.0110
L	8	27	8	27	8	27	29	44	77	116	–

[a] The number of function evaluations for all three PDD methods employing a full N-dimensional numerical integration and n-point univariate Gauss–Legendre rule is $L = n^N$, where $N=3$, $n=m+1$, and $1 \le m \le 2$.
[b] The results of PCE, including the numbers of function evaluations, were obtained from Sudret [9].
[c] The results of trivariate PDD for $m=2$ and PCE for $p=6$ coincide with the exact solution.
[d] The exact solution is $S_{\{i_1,\ldots,i_s\}} = 5^{-s}/[(6/5)^N - 1]$, $1 \le i_1 < \cdots < i_s \le N$, $s = 1, \ldots, N$, where $N=3$.

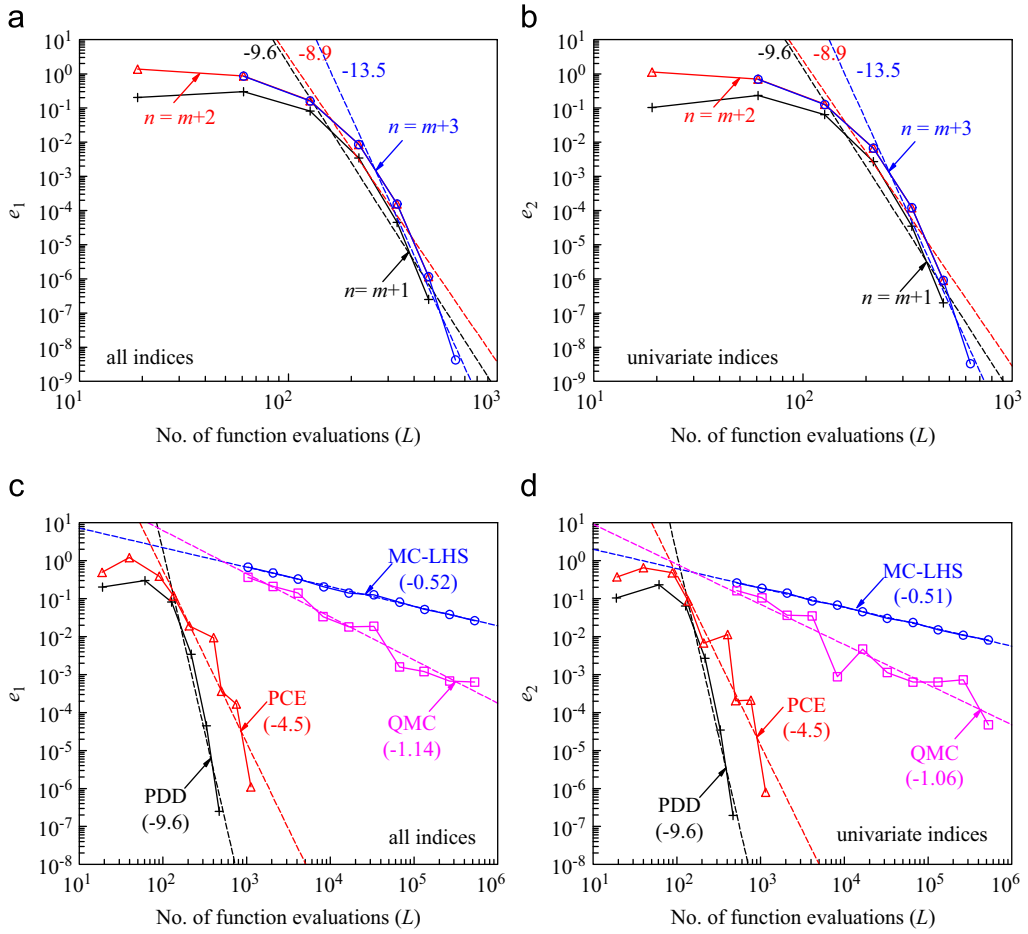

Fig. 2. $\mathcal{L}_1$-errors in calculating sensitivity indices of the Ishigami and Homma function (Example 2): (a) from all indices by PDD; (b) from univariate indices by PDD; (c) from all indices by various methods; and (d) from univariate indices by various methods. Note: the parenthetical values are slopes of the trend lines.

ascertain. Instead, three integration options, $n=m+1$ with $m=2,4,6,8,10,12$; $n=m+2$ with $m=1,3,5,7,9,11$; and $n=m+3$ with $m=2,4,6,8,10,12$, were employed to examine the influence of the option, if any, on the sensitivity indices. For each integration option, $1\le m\le 12$ was varied in such a way that n remained an odd integer. In so doing, the corresponding numbers (L) of function evaluations for a given m are $3m^2+3m+1$, $3(m+1)^2+3(m+1)+1$, and $3(m+2)^2+3(m+2)+1$, respectively.

Figs. 2(a) and (b) show how the errors e_1 and e_2, defined by Eqs. (32) and (33), from the bivariate PDD approximation vary with respect to L for all three integration options. The data points of these plots were generated by calculating the sensitivity indices for the selected values of m and counting the corresponding numbers of functions evaluations depending on the integration option. Ignoring the first two data points, the errors of PDD solutions from Figs. 2(a) and (b) decay proportionally to $L^{-9.6}$, $L^{-8.9}$, and $L^{-13.5}$ when $n=m+1$, $n=m+2$, and $n=m+3$, respectively. Clearly, their convergence rates – the absolute values of the slopes of the trend lines in the log–log plots – are much higher than unity for all three integration options. Figs. 2(c) and (d) compare the same two error measures from the bivariate PDD approximation ($n=m+1$) with those computed by Crestaux et al. [11] using the PCE, MC-LHS, and QMC methods or simulations. The sampling-based methods, MS-LHS and QMC, have convergence rates in the range of 0.51–1.14 and are no match for the PDD and PCE methods, which are endowed with significantly higher convergence rates, mostly due to the smoothness of y. Compared with PCE showing a convergence rate of 4.5, calculated ignoring also the first two data points in Figs. 2(c) and (d), the PDD approximation converges about twice as fast as the PCE approximation.[2] Although the same observation was made in Example 1, the validity of this trend depends on the function examined. More research is needed to establish appropriate criteria for grading these two methods.

5.3. Example 3: non-smooth function

In the third example, consider the non-smooth function

$$y(\boldsymbol{X})=\prod_{i=1}^{N}\frac{|4X_i-2|+a_i}{1+a_i} \tag{37}$$

of N independent and identically random variables X_i, $i=1,\ldots,N$, uniformly distributed on [0,1] and a_i, $i=1,\ldots,N$, are real-valued, non-negative, deterministic parameters. The lower the value of a_i, the greater the importance of X_i to y. Introduced by Saltelli and Sobol [32], this function has been widely used for benchmarking various sensitivity methods [9,11,33]. The exact solutions for variance and sensitivity indices are as follows: variance $\sigma^2=-1+\prod_{i=1}^{i=N}1+1/[3(1+a_i)^2]$ and sensitivity indices $S_{\{i_1,\ldots,i_s\}}=(1/\sigma^2)\prod_{p=1}^{p=s}1/[3(1+a_{i_p})^2]$, $1\le i_1<\cdots<i_s\le N$, $s=1,\ldots,N$.

The sensitivity analysis in this example was conducted for two problem sizes (dimensions): (1) $N=3$ with $a_1=0$, $a_2=1$, and

[2] A discrepancy exists between the convergence rates of PCE calculated in this paper and the value of 6 reported by Crestaux et al. [11]. This is possible because the number of data points used for calculating the convergence rate may differ. However, such discrepancy has no major implication on the conclusion.

$a_3=4.5$; and (2) $N=8$ with $a_1=0$, $a_2=1$, $a_3=4.5$, $a_4=9$, and $a_5=a_6=a_7=a_8=99$ [33]. When $N=3$ (low dimension), the trivariate PDD method ($S=3$) was employed to calculate the error e_2, the $\mathcal{L}_1$-error from the univariate indices only. The expansion coefficients for this low-dimensional problem were estimated using Legendre polynomials (interval$=[-1,+1]$) of orders $1\le m\le 12$ and full integration (Gauss–Legendre quadrature rule) with three integration options: $n=m+1$, $n=m+3$, and $n=m+5$. The plot of e_2 versus L, exhibited in Fig. 3, reveal an average convergence rate of 0.99, slightly varying with the integration option. Compared with the results of Example 2, the convergence rates in Example 3 have been significantly vitiated due to the lack of smoothness of y. Crestaux et al. [11] observed similar loss of convergence rates from the PCE method for the same function, however, with a different set of deterministic parameters. Therefore, both the PDD and PCE approximations are significantly challenged when faced with non-differentiable functions. In this example, the PDD method is on par with QMC simulation (asymptotic), which has a theoretical convergence rate of 1, and slightly better than MC-LHS (asymptotic), which has a theoretical convergence rate of 0.5.

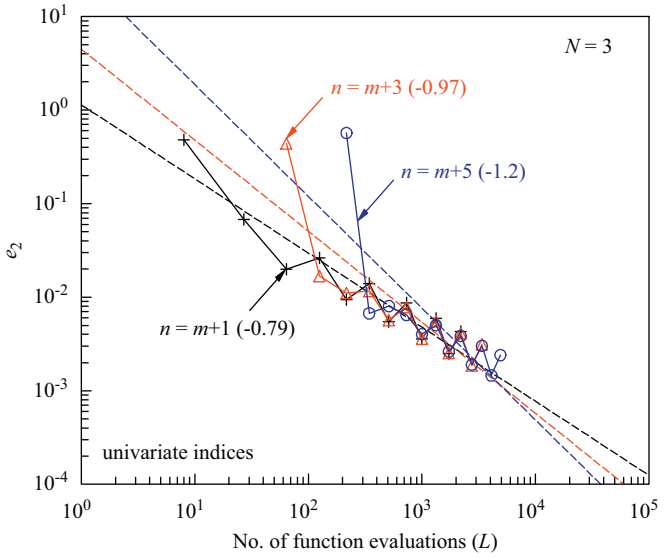

Fig. 3. $\mathcal{L}_1$-error in calculating univariate sensitivity indices of the non-smooth function ($N=3$) by PDD (Example 3). Note: the parenthetical values are slopes of the trend lines.

When $N=8$ (high dimension), the trivariate PDD approximation was applied again to compute the univariate sensitivity indices, $S_{\{i\}}$, $i=1,\ldots,8$, which are displayed in Table 2 along with their computational efforts. The expansion coefficients for this high-dimensional problem were estimated using Legendre polynomials (interval$=[-1,+1]$) of orders $m=4$ or $m=8$ and dimension-reduction integration (Gauss–Legendre quadrature rule) with $R=S=3$ and $n=m+1$. Since $3=S<N=8$, errors in calculating these indices occur not only due to a finite value of m (or n), but also due to the truncation of PDD. Table 2 also exhibits the univariate indices calculated by the RBD and SDP methods, analyzed by Gatelli et al. [33] for the same non-smooth function. For each of the two latter methods, two sets of results, one for a low sample size and the other for a high sample size, were selected in such a way that their computational efforts are closest to those required by the PDD method with the low and high values of polynomial order (m) selected. Therefore, the accuracy of a specific method, compared with the exact solution listed in Table 2, can be judged for similar computational efforts. From Table 2, all three methods for the largest polynomial order or sample size yield fairly accurate sensitivity indices due to highly important (X_1 and X_2) and slightly important (X_3 and X_4) input variables. In contrast, the SDP and PDD methods better estimate than the RBD method sensitivity indices due to unimportant (X_5-X_8) input variables, although predicting highly accurate sensitivities for unimportant variables is not crucial. From the analysis of Gatelli et al., the convergence rates of individual univariate sensitivity indices from the RBD and SDP methods vary from 0.41 to 1, approaching, at best, the theoretically achievable convergence rate of QMC simulation. Therefore, the RBD and SDP methods succumb to the same fate of the PDD approximation as well. Clearly, sensitivity analysis of non-smooth systems merits further study.

5.4. Example 4: Oakley and O'Hagan function

For Bayesian sensitivity analysis, Oakley and O'Hagan [34] introduced a mixture of trigonometric and quadratic polynomial functions, described by

$$y(\boldsymbol{X})=\boldsymbol{a}_1^T\boldsymbol{X}+\boldsymbol{a}_2^T\sin\boldsymbol{X}+\boldsymbol{a}_3^T\cos\boldsymbol{X}+\boldsymbol{X}^T\boldsymbol{M}\boldsymbol{X}, \tag{38}$$

where $\boldsymbol{X}=\{X_1,\ldots,X_{15}\}^T\in\mathbb{R}^{15}$ is a 15-dimensional standard Gaussian input vector ($N=15$) with mean vector $\mathbb{E}[\boldsymbol{X}]=\{0,\ldots,0\}^T=:\boldsymbol{0}\in\mathbb{R}^{15}$ and covariance matrix $\mathbb{E}[\boldsymbol{X}\boldsymbol{X}^T]=\mathrm{diag}[1,\ldots,1]=:\boldsymbol{I}\in\mathbb{R}^{15\times 15}$;

Table 2
Approximate and exact univariate sensitivity indices of the non-smooth function ($N=8$) by various methods (Example 3).

Sensitivity index & L	Trivariate PDD ($S=3$)[a]		RBD[b]		SDP[c]		Exact[d]
	$m=4$ ($n=5$)	$m=8$ ($n=9$)	Low sample size	High sample size	Low sample size	High sample size	
$\tilde{S}_{\{1\}},S_{\{1\}}$	0.7140	0.7218	0.704	0.714	0.717	0.716	0.7162
$\tilde{S}_{\{2\}},S_{\{2\}}$	0.1642	0.1723	0.173	0.181	0.179	0.179	0.1791
$\tilde{S}_{\{3\}},S_{\{3\}}$	0.0193	0.0207	0.0314	0.0278	0.0235	0.0236	0.0237
$\tilde{S}_{\{4\}},S_{\{4\}}$	0.0053	0.0057	0.0084	0.0073	0.0070	0.0071	0.0072
$\tilde{S}_{\{5\}},S_{\{5\}}$	4.8×10^{-5}	5.2×10^{-5}	4.4×10^{-3}	3.0×10^{-4}	2.1×10^{-5}	6.1×10^{-5}	7.2×10^{-5}
$\tilde{S}_{\{6\}},S_{\{6\}}$	4.8×10^{-5}	5.2×10^{-5}	3.8×10^{-3}	3.0×10^{-4}	2.3×10^{-5}	5.8×10^{-5}	7.2×10^{-5}
$\tilde{S}_{\{7\}},S_{\{7\}}$	4.8×10^{-5}	5.2×10^{-5}	2.2×10^{-3}	4.0×10^{-4}	2.2×10^{-5}	5.8×10^{-5}	7.2×10^{-5}
$\tilde{S}_{\{8\}},S_{\{8\}}$	4.8×10^{-5}	5.2×10^{-5}	1.7×10^{-3}	3.0×10^{-4}	2.0×10^{-5}	5.9×10^{-5}	7.2×10^{-5}
L	4065	30,529	4096	32,768	4096	32,768	–

[a] The number of function evaluations for the trivariate PDD method employing dimension-reduction integration with $R=S=3$ is $L=N(N-1)(N-2)(n-1)^3/6+N(N-1)(n-1)^2/2+N(n-1)+1$, where $N=8$, $n=m+1$, $4\le m\le 8$.
[b] RBD, random balance design [2]; the results were obtained from Gatelli et al. [33].
[c] SDP, state dependent parameter [5]; the results were obtained from Gatelli et al. [33].
[d] The exact solution is $S_{\{i\}}=(1/\sigma^2)/[3(1+a_i)^2]$, where $\sigma^2=-1+\prod_{i=1}^{i=N}1+1/[3(1+a_i)^2]$, $N=8$, and $a_1=0$, $a_2=1$, $a_3=4.5$, $a_4=9$, and $a_5=a_6=a_7=a_8=99$.

Table 3
Approximate and exact univariate sensitivity indices of the Oakley and O'Hagan function by various methods (Example 4).

Sensitivity index & L	Bivariate PDD ($S=2$)[a]			Exact[b]
	$m=2, n=3$	$m=4, n=5$	$m=6, n=7$	
$\tilde{S}_{\{1\}}, S_{\{1\}}$	0.001281	0.001541	0.001560	0.001560
$\tilde{S}_{\{2\}}, S_{\{2\}}$	0.000180	0.000189	0.000186	0.000186
$\tilde{S}_{\{3\}}, S_{\{3\}}$	0.001291	0.001308	0.001307	0.001307
$\tilde{S}_{\{4\}}, S_{\{4\}}$	0.003298	0.003046	0.003045	0.003045
$\tilde{S}_{\{5\}}, S_{\{5\}}$	0.003102	0.002908	0.002905	0.002905
$\tilde{S}_{\{6\}}, S_{\{6\}}$	0.022760	0.022991	0.023033	0.023035
$\tilde{S}_{\{7\}}, S_{\{7\}}$	0.024677	0.024141	0.024150	0.024151
$\tilde{S}_{\{8\}}, S_{\{8\}}$	0.026025	0.026528	0.026516	0.026517
$\tilde{S}_{\{9\}}, S_{\{9\}}$	0.049019	0.046071	0.046035	0.046036
$\tilde{S}_{\{10\}}, S_{\{10\}}$	0.014463	0.014942	0.014946	0.014945
$\tilde{S}_{\{11\}}, S_{\{11\}}$	0.104726	0.102020	0.101830	0.101823
$\tilde{S}_{\{12\}}, S_{\{12\}}$	0.131333	0.135520	0.135706	0.135708
$\tilde{S}_{\{13\}}, S_{\{13\}}$	0.099474	0.101985	0.101986	0.101989
$\tilde{S}_{\{14\}}, S_{\{14\}}$	0.103659	0.105201	0.105175	0.105169
$\tilde{S}_{\{15\}}, S_{\{15\}}$	0.118182	0.122687	0.122812	0.122818
L	451	1741	3871	–

[a] The number of function evaluations for the bivariate PDD method employing dimension-reduction integration with $R=S=2$ is $L=N(N-1)(n-1)^2/2+N(n-1)+1$, where $N=15$, $n=m+1$, $2\le m\le 6$.
[b] See Oakley and O'Hagan [34] or Gatelli et al. [33].

$\sin\boldsymbol{X} \coloneqq \{\sin X_1,\ldots,\sin X_{15}\}^T \in \mathbb{R}^{15}$ and $\cos\boldsymbol{X} \coloneqq \{\cos X_1,\ldots,\cos X_{15}\}^T \in \mathbb{R}^{15}$ are compact notations for 15-dimensional vectors of sine and cosine functions, respectively; and $\boldsymbol{a}_i \in \mathbb{R}^{15}$, $i=1,2,3$, and $\boldsymbol{M} \in \mathbb{R}^{15\times 15}$ are coefficient vectors and matrix, respectively, obtained from Oakley and O'Hagan's paper [34]. The coefficient vectors were selected so that the first five variables are unimportant, the next five variables are slightly important, and the last five variables are very important. The coefficient matrix reflects cooperative effects from all pairs of random variables. The exact solutions of 15 univariate sensitivity indices, obtained from Oakley and O'Hagan, are listed in Table 3. The three groups of input variables are clearly identified in increasing order of importance.

Although $y:\mathbb{R}^{15}\to\mathbb{R}$, each term on the right side of Eq. (38) includes at most bivariate combinations of random variables. Therefore, the bivariate PDD approximation ($S=2$) is adequate and was employed to calculate the univariate indices. The expansion coefficients were estimated using Hermite polynomials (interval $=[-\infty,+\infty]$) of orders $2\le m\le 6$ and dimension-reduction (Gauss–Hermite quadrature rule) integration with $R=S=2$ and $n=m+1$. Table 3 presents the univariate indices computed by the bivariate PDD method for three polynomial orders, $m=2$, $m=4$, and $m=6$, including the required numbers of function evaluations. When $m=2$ (lowest-order polynomial), there exist some discrepancy between the indices estimated by the PDD and the exact solutions, although the relative importance of input variables is clearly recognized already. When m increases, the accuracy of the estimated indices improves rapidly, however, with increased computational demand. When $m=6$, the largest polynomial order considered, the estimated indices are practically coincident with the exact solutions.

Gatelli et al. [33] also evaluated the error $e_{3,i}$, defined as the relative error in calculating each univariate sensitivity index $S_{\{i\}}$ (see Eq. (34)), for this problem using the RBD, SDP, and improved Sobol's method. They reported convergence rates varying from 0.2 to 0.92 for RBD (Figure 6 of Gatelli et al.), 0.43 to 0.61 for SDP (Figure 8 of Gatelli et al.), and 0.4 to 0.81 for improved Sobol's (Figure 7 of Gatelli et al.) methods, depending on the input variable examined.

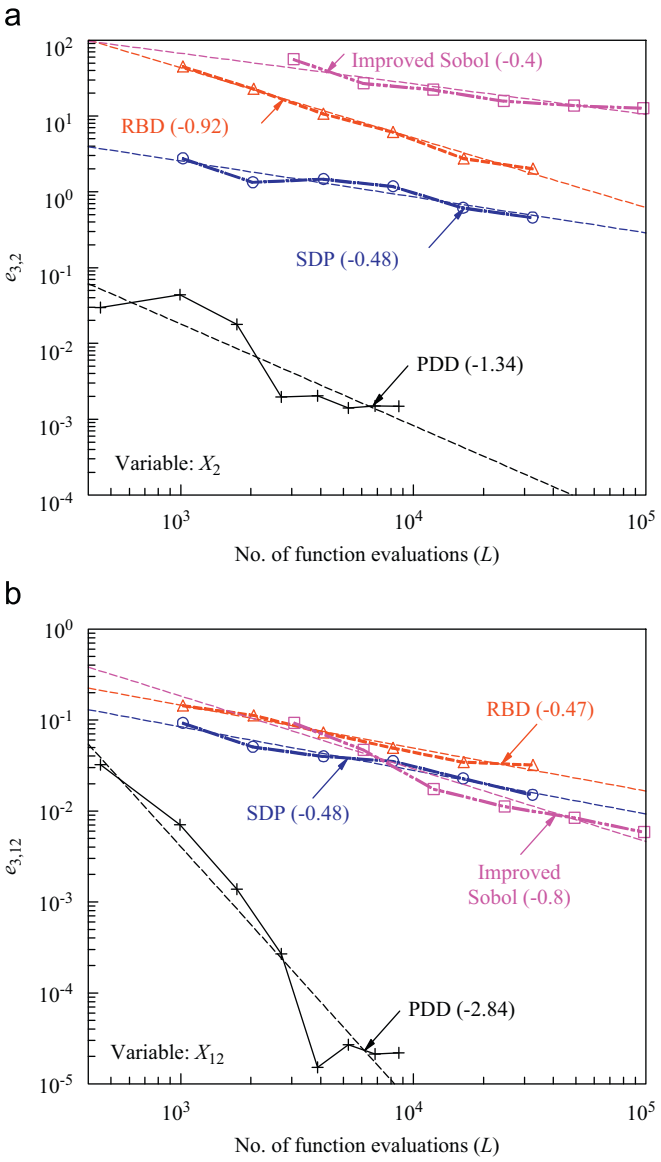

Fig. 4. Relative error in calculating individual univariate sensitivity indices of the Oakley and O'Hagan function by PDD (Example 4): (a) input variable X_2 and (b) input variable X_{12}. Note: the parenthetical values are slopes of the trend lines.

Therefore, the convergence behaviors of all three aforementioned methods are worse than QMC simulation (asymptotic), although the convergence rates of the RBD method for a few variables are close to 1. From the exact univariate indices in Table 3, $S_{\{2\}}$ and $S_{\{12\}}$ are the smallest and largest indices, respectively; therefore, X_2 is the least important variable, while X_{12} is the most important variable. Figs. 4(a) and (b) show the convergence curves for these two extreme variables, obtained from the bivariate PDD, RBD, SDP, and improved Sobol's method. The errors from the PDD approximation for a given number of function evaluations are significantly lower than those obtained from any of the three competing methods examined. The convergence rates of RBD, SDP, and improved Sobol's method, calculated using all data points in Figs. 4(a) and (b), are 0.92, 0.48[3], and 0.4, respectively, for $S_{\{2\}}$ and 0.47, 0.48, and 0.8,

[3] For the SDP method, Gatelli et al. [33] reported a value of 0.61 for $S_{\{2\}}$ in Figures 8 and 9 of their paper. However, the location of the fitted curves at $\log N=1000$ is slightly above the data point in Figure 8 and is slightly below the data point in Figure 9. Due to this discrepancy, the author conducted his own fit of the raw data, yielding a convergence rate of 0.48.

respectively, for $S_{\{12\}}$. In contrast, the convergence rates of the PDD approximation in estimating $S_{\{2\}}$ and $S_{\{12\}}$ are 1.34 and 2.84, respectively, and are much higher than those obtained from the other three methods. The relatively superior performance of PDD is due to the combination of the bivariate dimensional structure and smoothness properties of y. However, the convergence rates of the PDD method achieved in Example 4 have not been as high as the ones observed in Example 2. This is because of the larger number of random variables in this example, implying slight deterioration of the convergence properties with the dimension of the problem.

It is important to emphasize that estimating sensitivity indices by PCE with a target error close to those produced by the bivariate PDD with $m=6$ (fourth column of Table 3) would be a daunting task. This is because of the need to employ very high-order multivariate polynomials in 15 variables, generating extremely large number of PCE coefficients, not to mention the calculation of numerous high-dimensional integrals involved.

5.5. Example 5: leverarm stress analysis

The final example illustrates the PDD method for GSA of an industrial-scale, stochastic mechanics problem. It involves stress analysis of a leverarm in a wheel loader, depicted in Fig. 5(a), commonly used in the heavy construction industry. The loading and boundary conditions of a single leverarm are shown in Fig. 5(b). Fig. 5(c) presents an undeformed leverarm mesh from the ABAQUS commercial code [35], comprising 48,312 tetrahedral finite elements. Two random loads P_H and P_V acting at pin E can be viewed as input loads due to other mechanical components of the wheel loader. The essential boundary conditions, sketched in Fig. 5(b), define random prescribed displacements u_{xF} and u_{yF} at pin F and u_{xG}, and u_{yG} at pin G. The leverarm is made of cast steel with random Young's modulus E and random Poisson's ratio v. The input vector $\boldsymbol{X}=\{P_H,P_V,E,v,u_{xF},u_{yF},u_{xG},u_{yG}\}^T\in\mathbb{R}^8$ includes eight independent random variables with their statistical properties listed in Table 4. Both the univariate ($S=1$) and bivariate ($S=2$) PDD methods with measure-consistent orthogonal polynomials and Gauss quadrature rule derived from the Stieltjes procedure [24] were employed for sensitivity analysis of an elastic response from finite-element analysis (FEA) of the leverarm. The expansion coefficients were estimated by dimension-reduction integration with $R=S$, requiring one- or at most two-dimensional integrations. The order m of orthogonal polynomials and number n of integration points in the dimension-reduction integration are $2\le m\le 3$ and $n=m+1$, respectively.

Table 5 presents the approximate univariate sensitivity indices and second-moment statistics of the maximum von Mises stress

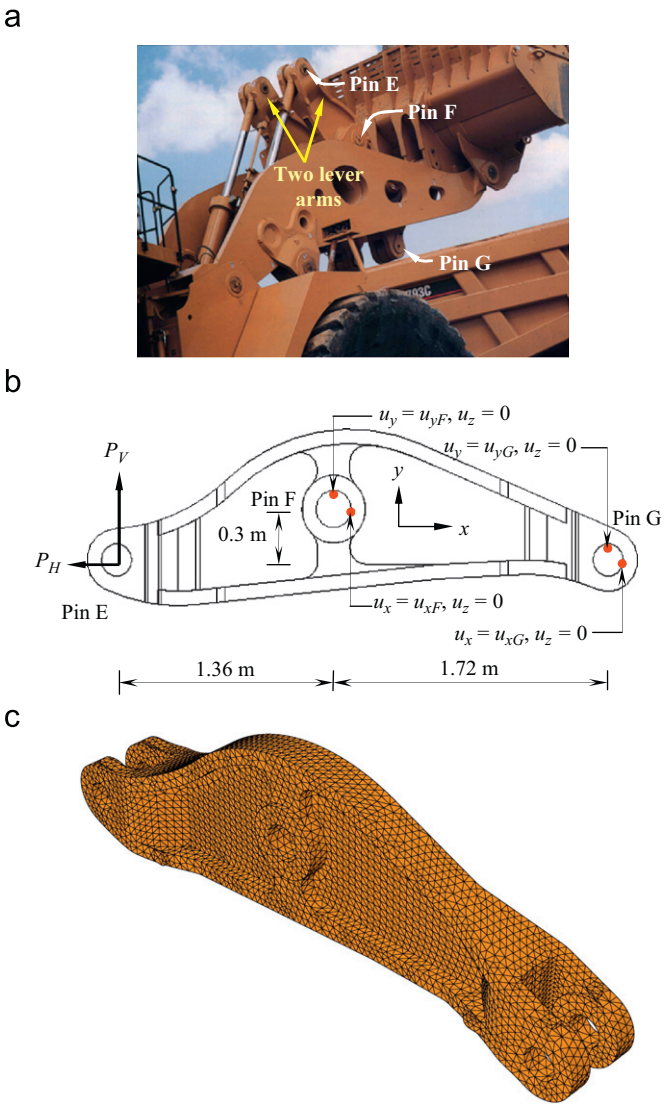

Fig. 5. Structural analysis of a leverarm: (a) two leverarms in a wheel loader; (b) geometry, loading, and boundary conditions; and (c) undeformed mesh (48,312 elements).

Table 4
Statistical properties of leverarm random input (Example 5).

Random variable	Mean	Standard deviation	Probability distribution
P_H[a] (kN)	507.69	76.15	Lognormal
P_V[a] (kN)	1517.32	227.60	Lognormal
E (GPa)	203	10.15	Lognormal
v	0.3	0.015	Lognormal
u_{xF} (mm)	−5	$5/\sqrt{3}$	Uniform[b]
u_{yF} (mm)	5	$5/\sqrt{3}$	Uniform[c]
u_{xG} (mm)	5	$5/\sqrt{3}$	Uniform[c]
u_{yG} (mm)	−5	$5/\sqrt{3}$	Uniform[b]

[a] To be distributed equally (halved) on front and back sides of pin E.
[b] Uniformly distributed over [−10,0] mm; to be applied on both sides.
[c] Uniformly distributed over [0,10] mm; to be applied on both sides.

Table 5
Approximate univariate sensitivity indices and second-moment statistics of the maximum von Mises stress in the leverarm by PDD methods (Example 5).

Sensitivity index, statistics & L	Univariate PDD ($S=1$)[a]		Bivariate PDD ($S=2$)[b]	
	$m=2$, $n=3$	$m=3$, $n=4$	$m=2$, $n=3$	$m=3$, $n=4$
$\tilde{S}_{\{1\}}$	2.82×10^{-4}	2.82×10^{-4}	2.81×10^{-4}	2.81×10^{-4}
$\tilde{S}_{\{2\}}$	0.0207	0.0207	0.0206	0.0206
$\tilde{S}_{\{3\}}$	0.0193	0.0193	0.0192	0.0186
$\tilde{S}_{\{4\}}$	3.53×10^{-5}	3.53×10^{-5}	3.52×10^{-5}	3.40×10^{-5}
$\tilde{S}_{\{5\}}$	0.4657	0.4657	0.4646	0.4651
$\tilde{S}_{\{6\}}$	0.0142	0.0142	0.0141	0.0141
$\tilde{S}_{\{7\}}$	0.4657	0.4657	0.4646	0.4651
$\tilde{S}_{\{8\}}$	0.0142	0.0142	0.0141	0.0137
Mean (MPa)	510.51	510.51	510.53	510.57
Variance (MPa^2)	17,604	17,604	17,658	17,668
L	25	33	277	481

[a] The number of function evaluations for the univariate PDD method employing dimension-reduction integration with $R=S=1$ is $L=Nn+1$, where $N=8$, $n=m+1$, $2\le m\le 3$.
[b] The number of function evaluations for the bivariate PDD method employing dimension-reduction integration with $R=S=2$ is $L=N(N-1)n^2/2+Nn+1$, where $N=8$, $n=m+1$, $2\le m\le 3$.

of the entire leverarm by the univariate and bivariate PDD methods. The von Mises stress is commonly used for examining material yielding or fatigue damage in mechanical systems. The sensitivity indices by the PDD methods in Table 5 quickly converge with respect to S and/or m. Since FEA is employed for response evaluations, the computational effort of PDD comes primarily from numerically determining the expansion coefficients. The expenses involved in estimating the PDD coefficients vary from 25–33 FEA for the univariate PDD and 277–481 FEA for the bivariate PDD, depending on the values of m. Based on the univariate indices in Table 5, the horizontal boundary conditions (u_{xF} and u_{xG}) are highly important; the vertical load (P_V), elastic modulus (E), and vertical boundary conditions (u_{yF} and u_{yG}) are slightly important; and the horizontal load (P_H) and Poisson's ratio (v) are unimportant in influencing the variance of the maximum von Mises stress.

Since no exact solution exists, crude Monte Carlo simulation up to 1000 realizations (FEA) was performed, estimating the mean and variance of the maximum von Mises stress to be 513.87 MPa and 17,956 MPa^2, respectively. They match very well with the approximate second-moment statistics in Table 5 from either version of the PDD method regardless of m (see Table 5), providing confidence on the accuracy of the indices computed by the PDD methods. The univariate solution is not only accurate, but also highly efficient. This is because of a realistic example chosen, where the individual effects of input variables on the response variance are dominant over their cooperative effects. Finally, this example demonstrates the non-intrusive nature of the PDD method, which can be easily integrated with external commercial codes for GSA of large-scale engineering systems.

6. Conclusions

A PDD method was developed for GSA of stochastic systems subject to independent random input following arbitrary probability distributions. The method is based on Fourier-polynomial expansions of lower-variate component functions of a stochastic response by measure-consistent orthonormal polynomial bases, analytical formulae for calculating the global sensitivity indices in terms of the expansion coefficients, and dimension-reduction integration for efficiently estimating the expansion coefficients. Compared with PCE, which contains the same orthonormal polynomials, but is arranged with respect to the order of polynomials, PDD is structured with respect to the degree of cooperativity between a finite number of random variables. As a result, PDD facilitates simple, direct, and immediate calculation of the global sensitivity indices without the need to generate the ANOVA decomposition of PCE. The PDD method employs measure-consistent orthogonal polynomials, sidestepping the need for transforming arbitrarily distributed random variables to uniform random variables, as required by the classical ANOVA decomposition. The computational complexity of the PDD method is polynomial, as opposed to exponential, consequently curbing the curse of dimensionality to some extent.

The PDD method was employed to calculate the global sensitivity indices in five numerical problems, where the output functions are various mathematical constructs involving smooth or non-smooth functions and complex responses from FEA. The error analyses indicate rapid convergence of the PDD solution for smooth non-polynomials, easily outperforming MC-LHS and QMC simulations. Moreover, from the results of the smooth functions examined, the convergence rates of the PDD method are noticeably higher than those of the PCE approximation and other competing methods, including RBD, SDP, and improved Sobol's methods. However, for non-smooth functions, there is a significant loss of convergence properties of the PDD approximation, eroding its advantage over existing methods. Therefore, further improvements of PDD are necessary to effectively deal with non-differentiable functions. The final example demonstrates how the PDD method can be integrated with an external FEA code, identifying important and unimportant variables during stress analysis of a complex mechanical system.

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References

[1] Saltelli A, Ratto M, Andres T, Campolongo F, Cariboni J, Gatelli D, et al. Global sensitivity analysis: the primer. West Sussex: Wiley; 2008.
[2] Tarantola S, Gatelli D, Mara TA. Random balance designs for the estimation of first-order global sensitivity indices. Reliability Engineering and System Safety 2006;91(l):717–27.
[3] Satterthwaite FE. Random balance experimentation. Technometrics 1959;1(2).
[4] Cukier RI, Levine HB, Shuler KE. Nonlinear sensitivity analysis of multiparameter model systems. Journal of Computational Physics 1978;26:1–42.
[5] Ratto M, Pagano A, Young P. State dependent parameter metamodelling and sensitivity analysis. Computer Physics Communications 2007;177:863–76.
[6] Sobol IM. Sensitivity analysis for nonlinear mathematical models. Mathematical Modelling & Computational Experiment 1993;1:407–14.
[7] Saltelli A. Making best use of model evaluations to compute sensitivity indices. Computer Physics Communications 2002;145:280–97.
[8] Saltelli A, Annoni P, Azzini I, Campolongo F, Ratto M, Tarantola S. Variance based sensitivity analysis of model output: design and estimator for the total sensitivity index. Computer Physics Communications 2010;181:259–70.
[9] Sudret B. Global sensitivity analysis using polynomial chaos expansions. Reliability Engineering and System Safety 2008;93(7):964–79.
[10] Ghanem RG, Spanos PD. Stochastic finite elements: a spectral approach. New York: Springer-Verlag; 1991.
[11] Crestaux T, Le Maitre O, Martinez JM. Polynomial chaos expansion for sensitivity analysis. Reliability Engineering and System Safety 2008;94(7):1161–72.
[12] Helton JC, Davis FJ. Latin hypercube sampling and the propagation of uncertainty in analyses of complex systems. Reliability Engineering and System Safety 2003;81(1):23–69.
[13] Sobol IM. On the distribution of points in a cube and the approximate evaluation of integrals. USSR Computational Mathematics and Mathematical Physics 1967;7(4):86–112.
[14] Hoeffding W. A class of statistics with asymptotically normal distributions. Annals of Mathematical Statistics 1948;19:293–325.
[15] Efron B, Stein C. The jackknife estimate of variance. Annals of Statistics 1981;9:586–96.
[16] Rabitz H, Alis O. General foundations of high dimensional model representations. Journal of Mathematical Chemistry 1999;25:197–233.
[17] Li G, Wang SW, Rabitz H. Practical approaches to construct RS-HDMR component functions. Journal of Physical Chemistry A 2002;106:8721–33.
[18] Rahman S, Xu H. A univariate dimension-reduction method for multidimensional integration in stochastic mechanics. Probabilistic Engineering Mechanics 2004;19:393–408.
[19] Xu H, Rahman S. A generalized dimension-reduction method for multidimensional integration in stochastic mechanics. International Journal for Numerical Methods in Engineering 2004;61:1992–2019.
[20] Xu H, Rahman S. Decomposition methods for structural reliability analysis. Probabilistic Engineering Mechanics 2005;20:239–50.
[21] Rahman S. Decomposition methods for structural reliability analysis revisited. Probabilistic Engineering Mechanic 2011;26:357–63.
[22] Sobol IM. Theorems and examples on high dimensional model representations. Reliability Engineering and System Safety 2003;79:187–93.
[23] Rahman S. A polynomial dimensional decomposition for stochastic computing. International Journal for Numerical Methods in Engineering 2008;76:2091–116.
[24] Rahman S. Extended polynomial dimensional decomposition for arbitrary probability distributions. Journal of Engineering Mechanics 2009;135(12):1439–51.
[25] Saltelli A, Tarantola S, Campolongo F, Ratto M. Sensitivity analysis in practice: a guide to assessing scientific models. John Wiley & Sons; 2004.
[26] Caflisch RE, Morokoff W, Owen A. Valuation of mortgage backed securities using Brownian bridges to reduce effective dimension. Journal of Computational Finance 1997;1:27–46.
[27] Rahman S. Statistical moments of polynomial dimensional decomposition. Journal of Engineering Mechanics 2010;136(7):923–7.

[28] Abramowitz M, Stegun IA. Handbook of mathematical functions. 9th ed. New York: Dover Publications Inc.; 1972.
[29] Rahman S, Yadav V. Orthogonal polynomial expansions for solving random eigenvalue problems. International Journal for Uncertainty Quantification 2011;1(2):163–87.
[30] Castillo E, Sánchez-Maroo N, Alonso A, Castillo C. Functional network topology learning and sensitivity analysis based on ANOVA decomposition. Neural Computation 2007;19(1):231–57.
[31] Ishigami T, Homma T. An importance quantification technique in uncertainty analysis for computer models. In: Proceedings of the ISUMA '90, first international symposium on uncertainty modeling and analysis, University of Maryland, 3–5 December; 1990. p. 398–403.
[32] Saltelli A, Sobol IM. About the use of rank transformation in sensitivity analysis of model output. Reliability Engineering and System Safety 1995; 50(3):225–39.
[33] Gatelli D, Kucherenko S, Ratto M, Tarantola S. Calculating first-order sensitivity measures: a benchmark of some recent methodologies. Reliability Engineering and System Safety 2009;94:1212–9.
[34] Oakley J, O'Hagan A. Probabilistic sensitivity analysis of complex models: a Bayesian approach. Journal of Royal Statistical Society: series B 2004;66:751–69.
[35] ABAQUS Standard, Version 6.9. Dassualt Systems Simulia Corp., Providence, RI, 2010.