Statistical Moments of Polynomial Dimensional Decomposition

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Abstract: This technical note presents explicit formulas for calculating the response moments of stochastic systems by polynomial dimensional decomposition entailing independent random input with arbitrary probability measures. The numerical results indicate that the formulas provide accurate, convergent, and computationally efficient estimates of the second-moment properties.

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Introduction

Dimensional decomposition splits a multivariate function into a finite sum of simpler component functions of input variables with increasing dimensions. The decomposition, first presented by Hoeffding (1948) in relation to his seminal work on *U*-statistics, has been studied by many other researchers, including Sobol (1969) for analysis of variance, Efron and Stein (1981) for jackknife estimate of variance, Rabitz and Alis (1999) for high-dimensional model representation, and Xu and Rahman (2005) for reliability analysis. More recently, the writer developed the polynomial dimensional decomposition (PDD) method involving Fourier-polynomial expansions of component functions (Rahman 2008), later extended for arbitrary probability measures (Rahman 2009), for stochastic computing.

This study further examines the writer's PDD method for calculating the response moments of a complex stochastic system. By exploiting the orthogonal structure of the decomposition and the properties of orthogonal polynomials, explicit formulas for calculating the response moments in terms of the expansion coefficients have been derived. The results of an industrial-scale leverarm example indicate that the formulas provide accurate, convergent, and computationally efficient estimates of the first two moments examined.

Polynomial Dimensional Decomposition

Let (Ω, \mathcal{F}, P) be a complete probability space, where Ω =sample space; $\mathcal{F}=\sigma$ -field on Ω ; and $P: \mathcal{F} \rightarrow [0,1]$ =probability measure. With \mathcal{B}^N representing the Borel σ -field on \mathbb{R}^N , consider an \mathbb{R}^N -valued independent random vector $X = \{X_1, \dots, X_N\}^T$: $(\Omega, \mathcal{F}) \rightarrow (\mathbb{R}^N, \mathcal{B}^N)$, which describes input to a complex stochastic system. The joint probability density function of X is $f_X(x) = \prod_{i=1}^{i=N} f_i(x_i)$, where $f_i(x_i)$ =marginal probability density function of X_i defined on the probability triple $(\Omega_i, \mathcal{F}_i, P_i)$. Let y(X), a real-valued, square-integrable, measurable transformation on (Ω, \mathcal{F}) , define a relevant response of the stochastic system. The PDD of y(X), described by (Rahman 2009)

$$y(X) = y_0 + \sum_{s=1}^{N} \left[\sum_{\substack{i_1=1 \\ s \text{ sums}}}^{N-s+1} \cdots \sum_{\substack{i_s=i_{s-1}+1 \\ s \text{ sums}}}^{N} \sum_{\substack{j_1=1 \\ s \text{ sums}}}^{\infty} \cdots \sum_{\substack{j_s=1 \\ s \text{ sums}}}^{\infty} C_{i_1\cdots i_s j_1\cdots j_s} \prod_{p=1}^{s} \psi_{i_p j_p}(X_{i_p}) \right]$$
(1)

can be viewed as a finite, hierarchical expansion of an output function in terms of its input variables with increasing dimensions, where { $\psi_{ij}(X_i)$, j=0,1,...} is a set of complete orthonormal bases in the Hilbert space $\mathcal{L}_2(\Omega_i, \mathcal{F}_i, P_i)$, which is consistent with the probability measure of X_i , and y_0 and $C_{i_1\cdots i_j j_1\cdots j_s}$, s = 1, 2, ..., N, are the expansion coefficients. In many applications, the function y in Eq. (1) can be approximated by a sum of at most S-variate component functions comprising at most m-order orthogonal polynomials, where $1 \le S \le N$ and $1 \le m \le \infty$ are both integers, resulting in the S-variate approximation (Rahman 2009)

$$\widetilde{y}_{S}(\boldsymbol{X}) = y_{0} + \sum_{s=1}^{S} \left[\sum_{\substack{i_{1}=1\\s \text{ sums}}}^{N-s+1} \cdots \sum_{\substack{i_{s}=i_{s-1}+1\\s \text{ sums}}}^{N} \sum_{j_{1}=1}^{m} \cdots \sum_{j_{s}=1}^{m} C_{i_{1}} \cdots i_{s} j_{1} \cdots j_{s}} \prod_{p=1}^{s} \psi_{i_{p}j_{p}}(X_{i_{p}}) \right]$$
(2)

which converges to $y(\mathbf{X})$ in the mean-square sense when S=N and $m \to \infty$. By minimizing an error functional associated with a given $y(\mathbf{x})$ and the joint probability density of $\{X_{i_1}, \ldots, X_{i_s}\}^T$, the coefficients can be expressed by the *N*-dimensional integrals (Rahman 2008)

$$y_0 = \int_{\mathbb{R}^N} y(\boldsymbol{x}) f_{\boldsymbol{X}}(\boldsymbol{x}) d\boldsymbol{x}$$
(3)

and

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$$C_{i_1\cdots i_s j_1\cdots j_s} = \int_{\mathbb{R}^N} y(\mathbf{x}) \prod_{p=1}^s \psi_{i_p j_p}(x_{i_p}) f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x}, \quad s = 1, 2, \dots, S$$
(4)

Once the embedded coefficients y_0 and $C_{i_1\cdots i_s j_1\cdots j_s}$, $s=1,2,\ldots,S$, are calculated, as described in the writer's previous work (Rahman 2009), Eq. (2) furnishes an approximate but explicit map $\tilde{y}_S: \mathbb{R}^N \to \mathbb{R}$ that can be viewed as a surrogate of the exact map $y: \mathbb{R}^N \to \mathbb{R}$, which describes the input-output relation from a complex numerical simulation. Therefore, any probabilistic characteristic of y(X), including its statistical moments and rare event probabilities, can be easily estimated by performing Monte Carlo simulation of $\tilde{y}_S(X)$ rather than of y(X). However, due to the special properties of orthogonal polynomials, explicit formulas for moments of $\tilde{y}_S(X)$ can be derived, and that is the principal focus of this work. Readers interested in tail distributions of response or reliability analysis are referred to prior works on PDD (Rahman 2008, 2009).

Orthogonal Polynomials

Let $f_i(x_i)$ be the probability density function of the random variable X_i under the probability measure $dF_i(x_i) = f_i(x_i)dx_i$, which has finite moments of orders up to $2m, m \in \mathbb{N}$. Let \mathbb{P} be the space of real polynomials and $\mathbb{P}_m \subset \mathbb{P}$ the space of polynomials of degree $\leq m$. For any pair $u_i(x_i), v_i(x_i)$ in \mathbb{P} , define an inner product

$$(u_{i}, v_{i})_{dF_{i}} \coloneqq \int_{\mathbb{R}} u_{i}(x_{i})v_{i}(x_{i})dF_{i}(x_{i}) = \int_{\mathbb{R}} u_{i}(x_{i})v_{i}(x_{i})f_{i}(x_{i})dx_{i} \quad (5)$$

and an associated norm $||u_i||_{dF_i} := \sqrt{(u_i, u_i)_{dF_i}}$ with respect to the measure $dF_i(x_i)$.

Definition: Monic real polynomials $\pi_{ij}(x_i) = x_i^j + \cdots, j$ =0,1,2,..., are called monic orthogonal polynomials with respect to the measure $dF_i(x_i)$ if

$$(\pi_{ij_1}, \pi_{ij_2})_{dF_i} = 0 \quad for \quad j_1 \neq j_2, \ j_1, j_2 = 0, 1, 2, \dots \quad and$$
$$\|\pi_{ij}\|_{dF_i} = \sqrt{(\pi_{ij}, \pi_{ij})_{dF_i}} > 0 \quad for \quad j = 0, 1, 2, \dots \quad (6)$$

There are infinitely many orthogonal polynomials if the index set $\{j=0,1,2,...\}$ is unbounded and finitely many otherwise.

Theorem: Let $\pi_{ij}(x_i)$, j=0,1,2,..., be monic orthogonal polynomials with respect to the measure $dF_i(x_i)$. They satisfy the three-term recurrence relation

$$\pi_{i,j+1}(x_i) = (x_i - a_{ij})\pi_{ij}(x_i) - b_{ij}\pi_{i,j-1}(x_i), \quad j = 0, 1, 2, \dots$$

$$\pi_{i,-1}(x_i) = 0, \quad \pi_{i0}(x_i) = 1$$
(7)

where

$$a_{ij} = \frac{(x_i \pi_{ij}, \pi_{ij})_{dF_i}}{(\pi_{ij}, \pi_{ij})_{dF_i}}, \quad j = 0, 1, 2, \dots$$
(8)

and

$$b_{ij} = \begin{cases} (\pi_{i0}, \pi_{i0})_{dF_i} & \text{if } j = 0\\ \frac{(\pi_{ij}, \pi_{ij})_{dF_i}}{(\pi_{i,j-1}, \pi_{i,j-1})_{dF_i}} & \text{if } j = 1, 2, \dots \end{cases}$$
(9)

are the recursion coefficients. The index range is infinite $(j \le \infty)$ or finite $(j \le m-1)$, depending on whether the inner product is

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positive definite on \mathbb{P} or \mathbb{P}_m , respectively, but not on $\mathbb{P}_{m'}$, m' > m.

Proof. See Gautschi (2004), pp. 10–13.

The three-term recurrence relation has significant impact on the construction of orthogonal polynomials. The first *m* recursion coefficient pairs are uniquely determined by the first 2m moments of X_i that must exist. When these moments can be exactly calculated, they lead to exact recursion coefficients, some of which belong to classical orthogonal polynomials. For an arbitrary measure, approximate methods based on the Stieltjes procedure can be employed to obtain the recursion coefficients. See Rahman (2009) for further details.

Let $\psi_{ij}(x_i) \coloneqq \pi_{ij}(x_i) / ||\pi_{ij}(x_i)||_{dF_i}$, j=0,1,2,..., define orthonormal versions of monic orthogonal polynomials for an arbitrary measure dF_i . If \mathbb{E} is the expectation operator, then two important properties of $\psi_{ij}(x_i)$ are as follows.

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

$$\mathbb{E}[\psi_{ij}(X_i)] \coloneqq \int_{\mathbb{R}} \psi_{ij}(x_i) f_i(x_i) dx_i = \begin{cases} 1 & \text{if } j = 0\\ 0 & \text{if } j \ge 1 \end{cases}$$
(10)

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

$$\mathbb{E}[\psi_{ij_1}(X_i)\psi_{ij_2}(X_i)] \coloneqq \int_{\mathbb{R}} \psi_{ij_1}(x_i)\psi_{ij_2}(x_i)f_i(x_i)dx_i = \begin{cases} 1 & \text{if } j_1 = j_2 \\ 0 & \text{if } j_1 \neq j_2 \end{cases}$$
(11)

The first property stems from the expression $\mathbb{E}[\pi_{ij}(X_i)] = \int_{\mathbb{R}} \pi_{ij}(x_i) f_i(x_i) dx_i = (\pi_{ij}, \pi_{i0})_{dF_i}$, which, according to the aforementioned definition and theorem, is *one* when j=0 and *zero* when $j \ge 1$. The second property follows directly from the definition and theorem.

Moments

Applying the expectation operator on Eq. (2) and noting Property 1, the mean

$$\mathbb{E}[\tilde{y}_{S}(X)] = y_{0} \tag{12}$$

of the *S*-variate approximation matches the exact mean in Eq. (3), regardless of *S*. Applying the expectation operator again, this time on $[\tilde{y}_{S}(X) - y_{0}]^{2}$, results in the approximate variance

$$\mathbb{E}[\tilde{y}_{S}(X) - y_{0}]^{2} = \sum_{s=1}^{S} \sum_{t=1}^{S} \left\{ \underbrace{\sum_{i_{1}=1}^{N-s+1} \cdots \sum_{i_{s}=i_{s-1}+1}^{N} \sum_{j_{1}=1}^{m} \cdots \sum_{j_{s}=1}^{m} \cdots \sum_{j_{s}=1}^{m} \cdots \sum_{i_{s}=1}^{m} \cdots \sum_{i_{s}=1}$$

which depends on S. The number of summations inside the brace of the right side of Eq. (13) is 2(s+t), where s and t=indices of the two outer summations. By virtue of Property 2 and independent coordinates of X

$$\mathbb{E}\left[\prod_{p=1}^{s} \psi_{i_p j_p}(X_{i_p}) \prod_{p=1}^{t} \psi_{k_p l_p}(X_{k_p})\right] = \prod_{p=1}^{s} \mathbb{E}[\psi_{i_p j_p}^2(X_{i_p})] = 1 \quad (14)$$

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

$$\mathbb{E}[\tilde{y}_{S}(\boldsymbol{X}) - y_{0}]^{2} = \sum_{s=1}^{S} \left(\sum_{\substack{i_{1}=1 \\ s \text{ sums}}}^{N-s+1} \cdots \sum_{\substack{i_{s}=i_{s-1}+1 \\ s \text{ sums}}}^{N} \sum_{\substack{j_{1}=1 \\ s \text{ sums}}}^{m} \cdots \sum_{\substack{j_{s}=1 \\ s \text{ sums}}}^{m} C_{i_{1}}^{2} \cdots i_{s} j_{1} \cdots j_{s} \right)$$
(15)

as the sum of squares of the expansion coefficients from the S-variate approximation of $y(\mathbf{x})$. Clearly, the approximate variance in Eq. (15) approaches the exact variance

$$\mathbb{E}[y(\mathbf{X}) - y_0]^2 = \sum_{s=1}^N \left(\sum_{\substack{i_1=1\\s \text{ sums}}}^{N-s+1} \cdots \sum_{\substack{i_s=i_{s-1}+1\\s \text{ sums}}}^N \sum_{j_1=1}^\infty \cdots \sum_{j_s=1}^\infty C_{i_1\cdots i_s j_1\cdots j_s}^2 \right)$$
(16)

when S=N and $m \rightarrow \infty$. The mean-square convergence of \tilde{y}_s is guaranteed as y and its component functions are all members of the associated Hilbert spaces. Therefore, Eqs. (12) and (15) provide useful formulas for calculating the approximate mean and variance of a general stochastic response. Compared with the past work (Rahman 2009), no simulation of $\tilde{y}_s(X)$ is required to estimate the second-moment statistics of y(X).

Can the same idea be extended to explore higher-order moments? For instance, applying the expectation operator on $[\tilde{y}_{S}(X)-y_{0}]^{r}$, where r= positive integer, yields the *r*th-order central moment

$$\mathbb{E}[\tilde{y}_{S}(X) - y_{0}]^{r} = \sum_{s_{1}=1}^{S} \cdots \sum_{s_{r}=1}^{S} \left(\sum_{i_{s_{1},1}=1}^{N-s_{1}+1} \cdots \sum_{i_{s_{1},s_{1}}=i_{s_{1},s_{1}-1}=1}^{N} \sum_{j_{s_{1},1}=1}^{m} \cdots \sum_{j_{s_{1},s_{1}}=1}^{m} \cdots \sum_{j_{s_{1},s_{1}}=1}^{m} \cdots \sum_{j_{s_{r},s_{r}}=1}^{m} \cdots$$

However, for r > 2, expressing the expectation on the right side of Eq. (17) in terms of the expansion coefficients is hardly simple. Furthermore, expectations of products containing more than two orthonormal random polynomials are required. It is vital to emphasize that the PDD, like the polynomial chaos expansion (Field and Grigoriu 2004), does not guarantee convergence of moments of orders greater than two.





Fig. 1. 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)

For statistically dependent random variables, a direct approach to 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.

Computational Expense

The *S*-variate approximation in Eq. (2) requires evaluation of the coefficients y_0 and $C_{i_1\cdots i_s j_1\cdots j_s}$, $s=1,\ldots,S$. If the coefficients are estimated by dimension-reduction integration (Rahman 2009) involving at most *R*-dimensional ($S \le R < N$) integration with an *n*-point quadrature rule, as employed here, the following deterministic responses (function evaluations) are required: y(c), $y(c_1,\ldots,c_{k_1-1},x_{k_1}^{(j_1)},c_{k_1+1},\ldots,c_{k_R-1},x_{k_R}^{(j_R)},c_{k_R+1},\ldots,c_N)$ for $k_1,\ldots,k_R=1,\ldots,N$ and $j_1,\ldots,j_R=1,\ldots,n$, where $\mathbf{c}=\{c_1,\ldots,c_N\}^T$

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Table 1. Statistical Properties of Leverarm Random Input

Random variable	Mean	Standard deviation	Probability distribution
P_H^{a} , kN	507.69	76.15	Lognormal
P_V^{a} , kN	1,517.32	227.60	Lognormal
E, GPa	203	10.15	Lognormal
ν	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

^aTo be distributed equally (halved) on front and back sides of pin E. ^bUniformly distributed over [-10, 0] mm; to be applied on both sides.

^cUniformly distributed over [0, 10] mm; to be applied on both sides.

 $=\mathbb{E}[X]$ is the mean input and the superscripts on the variables indicate corresponding integration points. As a result, the total cost for the S-variate PDD entails a maximum of $\sum_{k=0}^{k=R} \binom{N}{R-k} n^{R-k}$ function evaluations. For instance, the univariate PDD (S=R=1) and bivariate (S=R=2) PDD will require only nN+1 (linear in N or n) and $N(N-1)n^2/2+nN+1$ (quadratic in N or n) function evaluations, respectively. Therefore, the PDD methods employing dimension-reduction integration should be more efficient than crude Monte Carlo simulation for solving problems involving moderate numbers (say, less than a hundred) of random variables. For higher-dimensional problems with hundreds or thousands of random variables, the decomposition in Eq. (1) is still useful, but more efficient methods are needed to calculate the expansion coefficients. Regardless of the problem size, the cost of generating measure-consistent orthogonal polynomials and associated Gauss quadrature formulas in PDD are negligible when compared with the calculation of the expansion coefficients.

Numerical Example

Consider a leverarm in a wheel loader depicted in Fig. 1(a), which is commonly used in the heavy construction industry. The loading and boundary conditions of a single leverarm are shown in Fig. 1(b). An undeformed leverarm mesh from ABAQUS (Simulia, Inc. 2008), which comprises 48,312 tetrahedral elements, is presented in Fig. 1(c). 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. 1(b), define random prescribed displacements u_{xF} and u_{yF} at pin F and u_{xG} , and u_{vG} at pin G. The leverarm is made of cast steel with random Young's modulus E and random Poisson's ratio ν . The input vector $X = \{P_H, P_V, E, \nu, u_{xF}, u_{yF}, u_{xG}, u_{yG}\}^T \in \mathbb{R}^8$ includes eight independent random variables with the statistical properties listed in Table 1. Both univariate (S=1) and bivariate (S=2) PDD methods with measure-consistent orthogonal polynomials (Rahman 2009) were employed to obtain the secondmoment statistics of three elastic responses generated by linearelastic finite-element analysis (FEA) of the leverarm. The expansion coefficients were estimated by dimension-reduction integration with R=S, where R=reduced dimension, requiring oneor at most two-dimensional integrations (Rahman 2009). The order m of orthogonal polynomials and number n of integration points in the dimension-reduction integration are $1 \le m \le 3$ and n=m+1, respectively.

Table 2 presents the approximate means and standard deviations of maximum von Mises stress ($\sigma_{e,max}$), maximum largest principal strain ($\epsilon_{1,max}$), and maximum distortional energy density ($U_{d,max}$) of the entire leverarm by the univariate and bivariate PDD methods. These elastic responses are commonly used for examining material yielding or fatigue damage in mechanical systems. The second-moment statistics by the PDD methods in Table 2, calculated using Eqs. (12) and (15), quickly converge with respect to *S* and/or *m*. Compared with the past work (Rahman 2009), no simulation of $\tilde{y}_{S}(X)$ was needed or performed to gener-

 Table 2. Second-Moment Properties of Leverarm Elastic Responses by Various Methods

	PDD							
m	Univariate (S=1)			Bivariate (S=2)			Crude Monte Carlo ^c	
	Mean	Standard deviation	Number of FEA ^a	Mean	Standard deviation	Number of FEA ^b	Mean	Standard deviation
			Maximu	m von Mises stre	ss ($\sigma_{e,\max}$) (MPa)			
1	510.51	132.68	17	510.51	132.86	129	513.87	134.00
2	510.51	132.68	25	510.53	132.88	277		
3	510.51	132.68	33	510.57	132.92	481		
			Maximum la	argest principal str	rain ($\epsilon_{1,max}$) (percen	t)		
1	0.253	0.065	17	0.253	0.065	129	0.254	0.065
2	0.253	0.065	25	0.253	0.065	277		
3	0.253	0.065	33	0.253	0.065	481		
			Maximum dis	stortional energy of	density $(U_{d,\max})$ (MI	Pa)		
1	0.593	0.287	17	0.593	0.290	129	0.599	0.294
2	0.593	0.288	25	0.593	0.291	277		
3	0.593	0.288	33	0.593	0.291	481		

 ${}^{a}nN+1$, where N=8, n=m+1 (Rahman 2009).

 ${}^{b}N(N-1)n^{2}/2+nN+1$, where N=8, n=m+1 (Rahman 2009).

^cSample size=1,000.

ate these statistics. 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 17-33 FEA for the univariate PDD and 129-481 FEA for the bivariate PDD, depending on the values of m. Since no exact solution exists, crude Monte Carlo simulation was performed up to 1,000 realizations. Compared with the Monte Carlo-generated statistics, also listed in Table 2, both versions of the PDD method provide excellent estimates of means and standard deviations of all three responses at lower computational costs. 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 second-moment statistics of response are dominant over their cooperative effects. However, for higher-order moments or tail probabilities, not examined here, the univariate PDD may not be adequate; bivariate PDD entailing higher-order orthogonal polynomials may be required (Rahman 2008).

Conclusions

The PDD involving Fourier-polynomial expansions of lowerdimensional component functions was studied. By exploiting the orthogonal structure of the decomposition and the properties of orthogonal polynomials, explicit formulas for calculating the response moments in terms of the expansion coefficients were derived. The results of an industrial-scale leverarm problem indicate that the formulas provide accurate and convergent estimates of the first two moments examined at modest computational effort.

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