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Convergence Properties of Polynomial Chaos Approximations for L_2 Random Variables

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Abstract

Polynomial chaos (PC) representations for non-Gaussian random variables are infinite series of Hermite polynomials of standard Gaussian random variables with deterministic coefficients. For calculations, the PC representations are truncated, creating what are herein referred to as PC approximations. We study some convergence properties of PC approximations for L_2 random variables. The well-known property of mean-square convergence is reviewed. Mathematical proof is then provided to show that higher-order moments (*i.e.*, greater than two) of PC approximations may or may not converge as the number of terms retained in the series, denoted by n, grows large. In particular, it is shown that the third absolute moment of the PC approximation for a lognormal random variable does converge, while moments of order four and higher of PC approximations for uniform random variables do not converge. It has been previously demonstrated through numerical study (see [4]) that this lack of convergence in the higher-order moments can have a profound effect on the rate of convergence of the tails of the distribution of the PC approximation. As a result, reliability estimates based on PC approximations can exhibit large errors, even when n is large. The purpose of this report is not to criticize the use of polynomial chaos for probabilistic analysis but, rather, to motivate the need for further study of the efficacy of the method.

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Convergence Properties of Polynomial Chaos Approximations for L_2 Random Variables

1   Introduction

Let

$$X = g(W) \tag{1}$$

be a random variable, where W is a zero mean, unit variance Gaussian random variable, and $g\colon \mathbb{R} \to \mathbb{R}$ is a deterministic measurable mapping such that X has finite variance. Often, finite-dimensional series approximations for X, denoted by X_n, are used for calculations. In this case, it becomes necessary to study the convergence properties of a sequence of random variables $\{X_n,\ n \geq 1\}$ approximating X. In this document we study the convergence properties of the polynomial chaos (PC) approximation, a particular class of approximating random variables. The study is limited to the standard polynomial chaos by Wiener, *i.e.*, infinite series of Hermite polynomials of standard Gaussian random variables; the recent extensions of polynomial chaos to general orthogonal polynomial functions of non-Gaussian random variables, *e.g.*, [10], are not considered.

It is well-known that PC approximations for L_2 random variables exhibit mean-square convergence [5, 7]. Further, this condition implies that the sequence of PC approximations $\{X_n,\ n \geq 1\}$ converges to X in probability and in distribution. Mean-square convergence does not, however, imply anything about the convergence of moments of order greater than two. Herein, we provide mathematical proof that moments of order greater than two of PC approximations may or may not converge as n gets large. Three examples are considered. For example 1, X takes a lognormal distribution and we show that $\mathrm{E}[|X_n|^3]$ converges to $\mathrm{E}[|X|^3]$ as $n \to \infty$. For examples 2 and 3, we consider random variables that do not take values over the entire real line, and prove that $\mathrm{E}[|X_n|^p]$ does not converge to $\mathrm{E}[|X|^p]$, for $p \geq 4$, as $n \to \infty$.

The practical effects of these results can be significant. It has been demonstrated through numerical study (see [4]) that this lack of convergence in the higher-order moments can have a profound effect on the rate of convergence of the tails of the distribution of the PC approximation. As a result, reliability estimates based on PC approximations can be in error even for large n, and the magnitude of these errors remains largely unquantified. Therefore, an analyst must take care to ensure that n is sufficiently large to accomplish the accuracy requirements for a given application.

The purpose of this study is not to criticize the use of polynomial chaos approximations for probabilistic analysis but, rather, to motivate the need for further study on the convergence properties of the approach. An explicit connection between the properties of mapping g defined by Eq. (1) and the rate of convergence of reliability estimates using PC approximation X_n would be particularly useful.

We review the concepts of convergence as applied to a sequence of random variables in Section 2. At the end of the section, we present two theorems related to the convergence of moments of a sequence of random variables. These concepts are then applied to the polynomial chaos approximation in Section 3; the section concludes with three examples. Two appendices are provided that include some detailed calculations.

2   Convergence concepts

Let X and X_n, $n \geq 1$, be real-valued random variables defined on probability space $(\Omega, \mathcal{B}, P)$. The distribution functions of X and X_n are F and F_n, respectively. We review different modes of convergence, as well as relationships between convergent sequences of random variables, to facilitate a discussion on the convergence properties of PC approximations in a later section.

2.1   Modes of convergence

The convergence of the sequence of random variables $\{X_n, \ n \geq 1\}$ to X has various definitions depending on the way in which the difference between X_n and X is measured. We refer to these definitions as modes of convergence.

Mode 1 *The sequence $\{X_n, \ n \geq 1\}$ is said to converge almost surely (a.s.) to X, written $X_n \xrightarrow{\text{a.s.}} X$, if*

$$\lim_{n \to \infty} X_n(\omega) = X(\omega), \ \forall \omega \in \Omega \setminus A,$$

where $P(A) = 0$.

This is the strongest mode of convergence possible for a sequence of random variables.

Mode 2 *Sequence $\{X_n, \ n \geq 1\}$ converges to X in probability (i.p.), written $X_n \xrightarrow{\text{i.p.}} X$, if for any $\epsilon > 0$,*

$$\lim_{n \to \infty} P\left(|X_n - X| > \epsilon\right) = 0.$$

For Mode 3, we need the following definition:

Definition 1 *Let $F(x) = P(X \leq x)$, $x \in \mathbb{R}$, denote the distribution function of random variable X; we say $X \in L_p$, $p > 0$, if*

$$\mathrm{E}\left[|X|^p\right] = \int_{\mathbb{R}} |x|^p \, dF(x) < \infty.$$

Note that for the special cases of $p = 1$ and $p = 2$, $\mathrm{E}[|X|] < \infty$ and $\mathrm{E}[X^2] < \infty$, meaning that X has finite mean and variance, respectively.

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Mode 3 *Let $X \in L_p$, $p \geq 1$, and let $\{X_n,\ n \geq 1\}$ denote a sequence of random variables such that $X_n \in L_p$, $n \geq 1$. If*

$$\lim_{n \to \infty} \mathrm{E}\left[|X_n - X|^p\right] = 0,$$

we say $\{X_n,\ n \geq 1\}$ converges to X in the L_p–sense, or simply $\{X_n,\ n \geq 1\}$ exhibits L_p convergence (see [9], Section 6.5). We denote this by $X_n \xrightarrow{L_p} X$.

We often refer to the special case of $p = 2$ as mean-square convergence.

Mode 4 *The sequence $\{X_n,\ n \geq 1\}$ is said to converge in distribution to X, written $X_n \xrightarrow{\mathrm{d}} X$, if*

$$\lim_{n \to \infty} F_n(x) = F(x),$$

$\forall x \in \mathbb{R}$ such that $F(x)$ is continuous. Mode 4 is also referred to as weak convergence; one reason is because, as stated in [9], p. 251, "unlike convergence in probability or L_p convergence, convergence in distribution says nothing about the behavior of the random variables themselves and only comments on the behavior of the distribution functions of the random variables."

2.2 Connections between modes of convergence

We next summarize some useful well-known relationships between convergent sequences of random variables.

Connection 1 $X_n \xrightarrow{\mathrm{a.s.}} X$ *implies* $X_n \xrightarrow{\mathrm{i.p.}} X$ *(see [9], p. 171).*

Connection 2 $X_n \xrightarrow{\mathrm{i.p.}} X$ *implies* $X_n \xrightarrow{\mathrm{d}} X$ *(see [9], p. 267).*

Connection 3 $X_n \xrightarrow{L_p} X$ *implies* $X_n \xrightarrow{\mathrm{i.p.}} X$ *and* $X_n \xrightarrow{L_q} X$, *if $0 < q \leq p$ (see [9], p. 181).*

Connection 4 $X_n \xrightarrow{L_p} X$ *implies convergence of the moments up to, and including, order p, i.e., $\lim_{n \to \infty} \mathrm{E}[|X_n|^q] = \mathrm{E}[|X|^q]$, $1 \leq q \leq p$.*

By Connections 2 and 3, $X_n \xrightarrow{L_p} X$, for $p > 0$, implies $X_n \xrightarrow{\mathrm{d}} X$. The converse is not true in general. More complex connections between convergent sequences of random variables are possible; we first need two additional definitions:

Definition 2 *For $p \geq 1$ and $X_n \in L_p$, $n \geq 1$, if*

$$\lim_{\substack{n \to \infty \\ m \to \infty}} \mathrm{E}\left[|X_n - X_m|^p\right] = 0,$$

we say sequence $\{X_n, \; n \geq 1\}$ is L_p–Cauchy.

Definition 3 *For $p \geq 1$, the sequence $\{|X_n|^p, n \geq 1\}$ is uniformly integrable (u.i.) if (see [9], Section 6.5.1)*

$$\lim_{a \to \infty} \sup_{n \geq 1} \mathrm{E}[|X_n|^p \, 1(|X_n|^p > a)] = 0,$$

where $1(A) = 1$ if event A is true and zero otherwise.

We make use of the next two theorems in following sections on convergence properties of PC approximations for non-Gaussian random variables.

Theorem 1 *For $p \geq 1$ and $X_n \in L_p$, $n \geq 1$, the following are equivalent (see [9], Theorem 6.6.2):*

(i) *$\{X_n, n \geq 1\}$ is L_p-convergent;*
(ii) *$\{X_n, n \geq 1\}$ is L_p-Cauchy; and*
(iii) *$\{X_n, n \geq 1\}$ is convergent in probability and $\{|X_n|^p, n \geq 1\}$ is u.i.*

Theorem 2 *If $X_n \in L_p$ and $X \in L_p$ for some $p \geq 1$, and $\{X_n, \; n \geq 1\}$ converges to X in probability, the following are equivalent (see [3], Theorem 4.5.4):*

(i) *$\{|X_n|^p, \; n \geq 1\}$ is u.i.;*
(ii) *$X_n \xrightarrow{L_p} X$; and*
(iii) *$\lim_{n \to \infty} \mathrm{E}\left[|X_n|^p\right] = \mathrm{E}\left[|X|^p\right] < \infty.$*

3 Polynomial chaos

Polynomial chaos (PC) representations for non-Gaussian random variables are infinite series of Hermite polynomials of standard Gaussian random variables with deterministic coefficients. PC representations remain a topic of continued research because, among other features, they provide a framework suitable for computational simulation. For calculations, the PC representations are truncated, creating what is herein referred to as PC approximations.

3.1 PC Representation

Under the assumption that X has finite variance, the infinite series [5, 7]

$$X = \sum_{k \geq 0} \beta_k \, h_k(W) \tag{2}$$

constitutes the PC representation for X, where β_k are deterministic coefficients that must be determined, $W \sim N(0,1)$ is a zero-mean, unit-variance Gaussian random variable, and

$$h_k(W) = \sum_{j=0}^{[k/2]} (-1)^j \, \frac{k!}{(k-2j)! \, j! \, 2^j} \, W^{k-2j} \tag{3}$$

are 1-dimensional Hermite orthogonal polynomials, where $[n]$ denotes the largest integer less than or equal to n. Collection $\{h_k(W), \; k \geq 0\}$ has the following properties (see [2])

$$\mathrm{E}[h_i(W)] = \begin{cases} 1 & i = 0, \\ 0 & i = 1, \ldots, n. \end{cases} \tag{4a}$$

$$\mathrm{E}[h_i(W) \, h_j(W)] = \begin{cases} i! & i = j, \\ 0 & i \neq j. \end{cases} \tag{4b}$$

$$\mathrm{E}[h_i(W) \, h_j(W) \, h_k(W)] = \begin{cases} \dfrac{i! j! k!}{(s-i)!(s-j)!(s-k)!} & i+j+k = 2s; i, j, k \leq s, \\ 0 & \text{otherwise.} \end{cases} \tag{4c}$$

Assuming $\mathrm{E}[g(W) \, h_k(W)]$ can be calculated term by term for $k = 0, 1, \ldots,$

$$\mathrm{E}[g(W) \, h_k(W)] = \mathrm{E}\left[\sum_{i \geq 0} \beta_i \, h_i(W) \, h_k(W) \right]$$

$$= \sum_{i \geq 0} \beta_i \, \mathrm{E}[h_i(W) \, h_k(W)] = \beta_k \, k!$$

so that

$$\beta_k = \frac{1}{k!} \, \mathrm{E}[g(W) \, h_k(W)], \ \ k = 0, 1, \dots \tag{5}$$

The second-moment properties of X are given by

$$\mathrm{E}[X] = \sum_{k \geq 0} \beta_k \, \mathrm{E}[h_k(W)] = \beta_0,$$

$$\mathrm{E}[X^2] = \sum_{j,k \geq 0} \beta_j \, \beta_k \, \mathrm{E}[h_j(W) \, h_k(W)] = \sum_{k \geq 0} \beta_k^2 \, k!,$$

where it is permissible to interchange sum and expectation since the sums are known to converge ($X \in L_2$).

3.2   PC approximation

Define

$$X_n = \sum_{k=0}^{n} \beta_k \, h_k(W) \tag{6}$$

to be the n-term PC approximation for X, where β_k is given by Eq. (5). The second-moment properties of X_n are given by

$$\mathrm{E}[X_n] = \sum_{k=0}^{n} \beta_k \, \mathrm{E}[h_k(W)] = \beta_0,$$

$$\mathrm{E}[X_n^2] = \sum_{j,k=0}^{n} \beta_j \, \beta_k \, \mathrm{E}[h_j(W) \, h_k(W)] = \sum_{k=0}^{n} \beta_k^2 \, k!.$$

3.3   Mean-square convergence of PC approximations

It is known that, for any $X \in L_2$, the PC approximation for X exhibits L_2 convergence [5, 7]. This follows from:

$$\mathrm{E}[X_n \, X] = \sum_{j=0}^{n} \sum_{k \geq 0} \beta_j \, \beta_k \, \mathrm{E}[h_j(W) \, h_k(W)] = \sum_{k=0}^{n} \beta_k^2 \, k!$$

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so that

$$\lim_{n \to \infty} \mathrm{E}[(X_n - X)^2] = \mathrm{E}[X^2] + \lim_{n \to \infty} \left(\mathrm{E}[X_n^2] - 2\,\mathrm{E}[X_n\,X] \right)$$

$$= \sum_{k \geq 0} \beta_k^2\,k! + \lim_{n \to \infty} \left(\sum_{k=0}^{n} \beta_k^2\,k! - 2 \sum_{k=0}^{n} \beta_k^2\,k! \right)$$

$$= \lim_{n \to \infty} \sum_{k \geq n+1} \beta_k^2\,k!$$

$$= 0.$$

By Connection 3, $\{X_n,\ n \geq 1\}$ converges to X in probability and in distribution, and by Connection 4, we have

$$\lim_{n \to \infty} \mathrm{E}[|X_n|^p] = \mathrm{E}[|X|^p],\ 1 \leq p \leq 2.$$

Further, by Theorem 1, $\{X_n\}$ is L_2-Cauchy and $\{X_n^2\}$ is uniformly integrable.

3.4 Convergence of higher-order moments of PC approximations

Through a series of examples, will show that $\mathrm{E}[|X_n|^p]$ may or may not converge to $\mathrm{E}[|X|^p]$ for $p > 2$. In example 1, X is a lognormal random variable, and we prove that the third absolute moment of X_n does converge to the third absolute moment of X as $n \to \infty$. In examples 2 and 3, we consider PC approximations for random variables that do not take values over the entire real line, and prove that all moments of order greater than or equal to four of both approximations diverge as the number of terms retained in the approximation gets large. X has a "reflected Gaussian" distribution for example 2, *i.e.*, $X = |W|$, where $W \sim N(0,1)$, and X has a uniform distribution on bounded interval $[a, b]$ for example 3. A new proposition that is needed for examples 2 and 3 is presented prior to example 2; a proof of the proposition is also provided.

Example 1

Let

$$X = g(W) = \exp(W),\ W \sim N(0,1). \tag{7}$$

By Eq. (7), random variable X has distribution $F(x) = \Phi(\ln x)$, $x > 0$, where $\Phi(\cdot)$ denotes the CDF of a $N(0,1)$ random variable, and moments $\mathrm{E}[|X|^p] = \mathrm{E}[X^p] = \exp(p^2/2) < \infty$, for $0 \leq p < \infty$. Because $\mathrm{E}[X^2] < \infty$, this particular $g(W)$ admits a PC representation.

Let Eq. (6) define the n-term PC approximation for X, where (see [4])

$$\beta_k = \frac{1}{k!} \operatorname{E}\left[\exp\left(W\right) h_k(W)\right] = \frac{1}{\sqrt{2\pi}\, k!} \int_{-\infty}^{\infty} \exp\left(u - \frac{u^2}{2}\right) h_k(u)\, \mathrm{d}u = \frac{1}{k!}\, e^{1/2} \qquad (8)$$

are the defining PC coefficients for $k = 0, 1, \ldots, n$. The third absolute moment of the n-term PC approximation for X is

$$
\begin{aligned}
\operatorname{E}[|X_n|^3] &= \operatorname{E}\left[\left|\sum_{k=0}^{n} \beta_k\, h_k(W)\right|^3\right] \\
&= \sum_{i,j,k=0}^{n} \beta_i\, \beta_j\, \beta_k\, \left|\operatorname{E}[h_i(W)\, h_j(W)\, h_k(W)]\right| \\
&= \sum_{\substack{i,j,k=0 \\ i+j+k=2s \\ i,j,k \le s}}^{n} e^{3/2}\, \frac{1}{i!\, j!\, k!}\, \frac{i!\, j!\, k!}{(s-i)!\,(s-j)!\,(s-k)!} \\
&= e^{3/2} \sum_{\substack{i,j,k=0 \\ i+j+k=2s \\ i,j,k \le s}}^{n} \frac{1}{(s-i)!\,(s-j)!\,(s-k)!} \\
&= e^{3/2} \sum_{\alpha=0}^{n} \frac{1}{\alpha!} \sum_{\beta=0}^{n-\alpha} \frac{1}{\beta!} \sum_{\gamma=0}^{n-\alpha-\beta} \frac{1}{\gamma!}
\end{aligned}
$$

where the second line follows because each $\beta_k > 0$, and the third line follows from Eq. (4c). Taking the limit, we have

$$
\begin{aligned}
\lim_{n\to\infty} \operatorname{E}[|X_n|^3] &= \lim_{n\to\infty} e^{3/2} \sum_{\alpha=0}^{n} \frac{1}{\alpha!} \sum_{\beta=0}^{n-\alpha} \frac{1}{\beta!} \sum_{\gamma=0}^{n-\alpha-\beta} \frac{1}{\gamma!} \\
&= e^{3/2}\,(e \cdot e \cdot e) = e^{9/2} = \operatorname{E}[|X|^3].
\end{aligned}
$$

The following proposition is needed for examples 2 and 3:

Proposition 1 *Let X_n denote the n-term PC approximation for random variable $X \in L_4$ and let*

$$a_n = \mathrm{E}\left[(X_n - X_{n-1})^4\right] = \beta_n^4 \, \mathrm{E}\left[h_n(W)^4\right].$$

If $\lim_{n\to\infty} a_n = \infty$, then $\mathrm{E}[|X_n|^p]$ does not converge to $\mathrm{E}[|X|^p]$ for $p \geq 4$.

Proof:

1. *By Theorem 1, sequence $\{|X_n|^4\}$ is not uniformly integrable. This follows because:*

   - *If sequence a_n does not converge, sequence $\{X_n\}$ is not L_4–Cauchy;*

   - *Any PC approximation exhibits L_2 convergence so that, by Connection 3, $X_n \xrightarrow{\text{i.p.}} X$; and*

   - *$X_n \in L_4$ for each $n \geq 0$ because it is a polynomial function of W.*

2. *By Theorem 2, $\lim_{n\to\infty} \mathrm{E}\left[X_n^4\right] \neq \mathrm{E}\left[X^4\right]$.*

3. *By the completeness of L_p spaces, $\lim_{n\to\infty} \mathrm{E}\left[|X_n|^p\right] \neq \mathrm{E}\left[|X|^p\right]$, $p > 4$.*

This completes the proof. □

Example 2

Let

$$X = g(W) = |W|, \ W \sim N(0,1). \tag{9}$$

By Eq. (9), random variable X has distribution $F(x) = \Phi(x) - \Phi(-x)$, $x \geq 0$, and moments

$$\mathrm{E}\left[|X|^p\right] = \frac{1}{\sqrt{2\pi}} \int_{\infty}^{\infty} |x|^p \exp\left(-x^2/2\right) \mathrm{d}x = \frac{2}{\sqrt{2\pi}} \int_0^{\infty} x^p \exp\left(-x^2/2\right) \mathrm{d}x$$

$$= \frac{2^{(p+1)/2}}{\sqrt{2\pi}} \Gamma\left(\frac{p+1}{2}\right) < \infty. \tag{10}$$

By Eq. (10), $X \in L_2$ so this particular $g(W)$ admits a PC representation.

Let Eq. (6) define the n-term PC approximation for X, where (see Appendix A)

$$\beta_{2k} = \frac{(-1)^{k-1}}{\sqrt{2\pi}\, 2^{k-1}\, (2k-1)\, k!}$$

$$\beta_{2k+1} = 0 \tag{11}$$

are the defining PC coefficients for $k = 0, 1, \ldots, n$. Because all odd coefficients vanish, it is sufficient to study

$$X_{2n} = \sum_{k=0}^{n} \beta_{2k}\, h_{2k}(W).$$

In [4], we observed by numerical studies that $E[X_n^4]$ did not approach $E[X^4]$ for $n \leq 20$; herein, we provide mathematical proof that $E[X_n^4]$ does not converge to $E[X^4]$ as $n \to \infty$. To do so, we construct sequence

$$a_{2n} = E\left[(X_{2n} - X_{2(n-1)})^4\right] = \beta_{2n}^4\, E\left[h_{2n}(W)^4\right]$$

and show that $\lim_{n \to \infty} a_{2n} = \infty$; this is sufficient by Proposition 1.

By Eq. (11) and Stirling's asymptotic relation for $n!$ (see [1], p. 257), we have

$$\beta_{2n}^4 \sim \left(\frac{e^n}{2\pi\, 2^{n-1}\, (2n-1)\, n^{n+1/2}}\right)^4 = \frac{e^{4n}}{\pi^4\, (2n)^{4n}\, n^2\, (2n-1)^4} \quad (\text{as } n \to \infty).$$

We next apply the Stirling formula to the lower bound for $E\left[h_{2n}(W)^4\right]$ derived in Appendix C (Eq. (16)) to show

$$E\left[h_{2n}(W)^4\right] \geq (4n)! \sim \sqrt{\pi}\, 2^{8n+3/2}\, n^{4n+1/2}\, e^{-4n} \quad (\text{as } n \to \infty).$$

It follows that

$$
\begin{aligned}
\lim_{n \to \infty} a_{2n} &= \lim_{n \to \infty} \beta_{2n}^4\, E\left[h_{2n}(W)^4\right] \\
&\geq \lim_{n \to \infty} \beta_{2n}^4\, (4n)! \\
&= \lim_{n \to \infty} \left(\frac{e^{4n}}{\pi^4\, (2n)^{4n}\, n^2\, (2n-1)^4}\right)\left(\sqrt{\pi}\, 2^{8n+3/2}\, n^{4n+1/2}\, e^{-4n}\right) \\
&= \frac{2^{3/2}}{\pi^{7/2}} \lim_{n \to \infty} \frac{2^{4n}}{n^{3/2}\, (2n-1)^4} \\
&= \infty
\end{aligned}
$$

where the last line follows by application of l'Hôpital's rule.

Example 3

Let X have a uniform distribution over $[a, b]$, *i.e.*,

$$X = g(W) = a + (b - a) \, \Phi(W), \; W \sim N(0, 1), \tag{12}$$

where $\Phi(\cdot)$ denotes the CDF of an $N(0, 1)$ random variable. By Eq. (12), random variable X has distribution $F(x) = (x - a)/(b - a)$, $a \leq x \leq b$, and moments

$$\mathrm{E}[|X|^p] = \int_a^b \frac{|x|^p}{b - a} \, \mathrm{d}x = \frac{1}{(b - a)(p + 1)} \left[\mathrm{sgn}(b) \, |b|^{p+1} - \mathrm{sgn}(a) \, |a|^{p+1} \right] < \infty, \tag{13}$$

where $\mathrm{sgn}(x) = x/|x|$, $x \neq 0$, is the sign of x. Because $\mathrm{E}[X^2] < \infty$, this particular $g(W)$ admits a PC representation.

Let Eq. (6) define the n-term PC approximation for X, where (see Appendix B)

$$\beta_0 = \frac{a + b}{2}, \quad \beta_{2k} = 0, \; k = 1, \ldots, n$$

$$\beta_{2k+1} = (-1)^k \frac{(b - a) \, (2k)!}{2^{2k+1} \sqrt{\pi} \, (2k + 1)! \, k!}, \quad k = 0, 1, \ldots, n \tag{14}$$

are the defining PC coefficients. Because all even coefficients greater than β_0 vanish, it is sufficient to study

$$X_{2n+1} = \sum_{k=0}^{n} \beta_{2k+1} \, h_{2k+1}(W).$$

We construct sequence

$$c_{2n+1} = \mathrm{E}\left[(X_{2n+1} - X_{2(n-1)+1})^4 \right] = \beta_{2n+1}^4 \, \mathrm{E}\left[h_{2n+1}(W)^4 \right]$$

and show that $\lim_{n \to \infty} c_{2n+1} = \infty$; this is sufficient to prove that $\mathrm{E}[|X_n|^p]$ does not converge to $\mathrm{E}[|X|^p]$ for $p \geq 4$ by Proposition 1.

By Eq. (14) and Stirling's asymptotic relation for $n!$ (see [1], p. 257), we have

$$\beta_{2n+1}^4 = \frac{(b - a)^4 \, ((2n)!)^4}{2^{4(2n+1)} \, \pi^2 \, ((2n + 1)!)^4 \, (n!)^4} = \frac{(b - a)^4}{2^{8n+4} \, \pi^2 \, (2n + 1)^4 \, (n!)^4}$$

$$\sim \frac{(b - a)^4 \, e^{4n}}{2^{8n+6} \, \pi^4 \, (2n + 1)^4 \, n^{4n+2}} \quad (\text{as } n \to \infty).$$

We next apply the Stirling formula to the lower bound for $\mathrm{E}\left[h_{2n+1}(W)^4 \right]$ derived in Appendix C (Eq. (17)) to show

$$\mathrm{E}\left[h_{2n+1}(W)^4 \right] \geq 2 \frac{(2n + 1)^5 \, ((2n)!)^5}{(n!)^6 \, (n + 1)^3} \sim \frac{2^{10n+3} \, n^{4n} \, (2n + 1)^5 \, e^{-4n}}{(n + 1)^3 \, \sqrt{\pi \, n}} \quad (\text{as } n \to \infty).$$

It follows that

$$\lim_{n\to\infty} c_{2n+1} = \lim_{n\to\infty} \beta_{2n+1}^4 \, \mathrm{E}\left[h_{2n+1}(W)^4\right]$$

$$\geq \lim_{n\to\infty} 2\,\beta_{2n+1}^4 \, \frac{(2n+1)^5 \, ((2n)!)^5}{(n!)^6 \, (n+1)^3}$$

$$= \lim_{n\to\infty} \left(\frac{(b-a)^4 \, e^{4n}}{2^{8n+6} \, \pi^4 \, (2n+1)^4 \, n^{4n+2}}\right) \left(\frac{2^{10n+3} \, n^{4n} \, (2n+1)^5 \, e^{-4n}}{(n+1)^3 \, \sqrt{\pi n}}\right)$$

$$= \frac{(b-a)^4}{8 \, \pi^{9/2}} \lim_{n\to\infty} \frac{2^{2n} \, (2n+1)}{n^{5/2} \, (n+1)^3}$$

$$= \infty$$

where the last line follows by application of l'Hôpital's rule.

Discussion

The fourth moment of the n-term PC approximation for X, *i.e.*, $\mathrm{E}[X_n^4]$, is shown in Fig. 1(a) over $0 \leq n \leq 40$. Results for both examples 2 and 3 are shown and, as proved above, both exhibit diverging behavior for large n. Further, $\mathrm{E}[X_n^4]$ for example 2 grows large at a faster rate than it does for example 3. For calculations, we set the range of X in example 3 to $[a, b] = [0, 1]$.

The practical effects of these results are illustrated by Fig. 1(b), which shows estimates of the corresponding tails of the distributions of X_n at the 1%-upper fractile, *i.e.*, estimates of $P(X_n \leq F^{-1}(0.99))$. Results from 100,000 Monte Carlo samples were used for calculations. Reliability estimates using the PC approximation for example 2 converge slowly when compared to the corresponding estimates for example 3; the latter exhibits negligible error for $n > 15$, while the former exhibits significant error for $n = 20$. Together, results illustrated by Fig. 1(a) and (b) suggest that, for the examples considered, the lack of converging fourth-order moments leads to slowly converging reliability estimates. Further, the faster these moments diverge, the less accurate a reliability estimate will be for a fixed n.
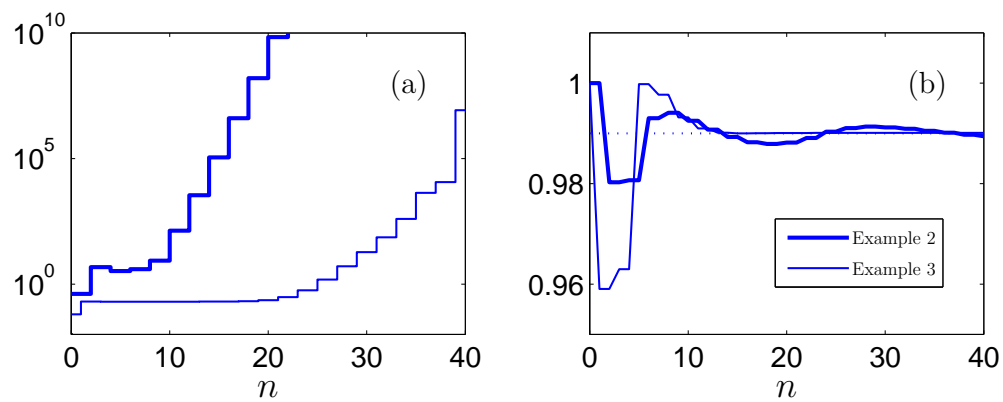
Figure 1. Plots of: (a) $E[X_n^4]$ and (b) estimates of the 1%-upper fractile as a function of n for examples 2 and 3 (taken from [4]).

4   Conclusions

We presented some convergence properties of general real-valued random variables, then utilized these properties to make observations regarding polynomial chaos (PC) approximations for L_2 random variables. Mathematical proof was supplied to show that higher-order moments (*i.e.*, greater than two) of PC approximations may or may not converge as the number of terms retained in the series, n, grows large. In particular, it was shown that the third absolute moment of the PC approximation for a lognormal random variable does converge, while moments of order four and higher of PC approximations for uniform random variables do not converge.

It was also demonstrated through numerical study that this lack of convergence of the higher-order moments can have a profound effect on the rate of convergence of the tails of the distribution of the PC approximation. Therefore, when using PC approximations for reliability calculations, one should take steps to ensure sufficient accuracy for the application is attained.

The purpose of this study was not to criticize the use of polynomial chaos approximations for probabilistic analysis but, rather, to motivate the need for further study on the convergence properties of the approach. A connection between the properties of mapping g defined by Eq. (1) and the rate of convergence of reliability estimates using PC approximation X_n would be particularly useful.

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A PC coefficients for $X = |W|$

By Eqs. (5) and (9),

$$\beta_k = \frac{1}{k!} \, \mathrm{E}\left[g(W) \, h_k(W)\right] = \frac{1}{\sqrt{2\pi} \, k!} \int_{-\infty}^{\infty} e^{-u^2/2} \, h_k(u) \, |u| \, \mathrm{d}u$$

$$= \begin{cases} \dfrac{2}{\sqrt{2\pi} \, k!} \displaystyle\int_0^{\infty} e^{-u^2/2} \, h_k(u) \, u \, \mathrm{d}u, & k = 0, 2, 4, \ldots \\ 0, & k = 1, 3, 5, \ldots \end{cases}$$

Let

$$b_{2k} = \int_0^{\infty} e^{-u^2/2} \, h_{2k}(u) \, u \, \mathrm{d}u = \frac{1}{2^{k-1}} \int_0^{\infty} e^{-v^2} \, \bar{h}_{2k}(v) \, v \, \mathrm{d}v,$$

where $\bar{h}_{2k}(x) = 2^k \, h_{2k}(\sqrt{2}x)$ is a modified set of orthogonal Hermite polynomials. By [6], p. 797, Eq. (7.376.2)

$$b_{2k} = (-1)^k \, \frac{2^{2k-2} \, \Gamma(1) \, \Gamma(k + 1/2) \, \Gamma(1/2) \, \Gamma(k - 1/2)}{\sqrt{\pi} \, 2^{k-2} \, \Gamma(k + 1/2) \, \Gamma(-1/2)}$$

$$= (-1)^{k-1} \, \frac{2^{k-1} \Gamma(k - 1/2)}{\sqrt{\pi}}$$

$$= (-1)^{k-1} \, \frac{(2k)!}{2^k \, k! \, (2k - 1)}$$

where the last step follows from [6], p. 888, Eq. (8.339.2). Hence,

$$\beta_{2k} = \frac{2}{\sqrt{2\pi} \, (2k)!} \, b_{2k} = \frac{(-1)^{k-1}}{\sqrt{2\pi} \, 2^{k-1} \, (2k - 1) \, k!}$$

which is consistent with Eq. (11).

B PC coefficients for X uniform on $[a, b]$

By Eqs. (5) and (12),

$$\beta_k = \frac{1}{k!} \, \mathrm{E}\left[g(W)\, h_k(W)\right] = \frac{1}{\sqrt{2\pi}\, k!} \int_{-\infty}^{\infty} e^{-u^2/2}\, h_k(u)\, (a + (b-a)\,\Phi(u))\, \mathrm{d}u$$

$$= \frac{1}{\sqrt{2\pi}\, k!} \int_{-\infty}^{\infty} e^{-u^2/2}\, h_k(u)\, \left(\frac{b-a}{2}\,\mathrm{erf}\left(\frac{u}{\sqrt{2}}\right)\right)\,\mathrm{d}u + \frac{b+a}{2\sqrt{2\pi}\, k!} \int_{-\infty}^{\infty} e^{-u^2/2}\, h_k(u)\,\mathrm{d}u$$

$$= I_{1,k} + I_{2,k}$$

where $\mathrm{erf}(x) = 2\,\Phi(\sqrt{2}x) - 1$ denotes the standard error function. By symmetry arguments, $I_{1,2k} = 0$, $k = 0, 1, \ldots$, and

$$I_{1,2k+1} = \frac{2}{\sqrt{2\pi}\,(2k+1)!} \int_0^{\infty} e^{-u^2/2}\, h_{2k+1}(u)\, \left(\frac{b-a}{2}\,\mathrm{erf}\left(\frac{u}{\sqrt{2}}\right)\right)\,\mathrm{d}u$$

$$= \frac{b-a}{\sqrt{2\pi}(2k+1)!\, 2^k} \int_0^{\infty} e^{-v^2}\, \bar{h}_{2k+1}(v)\,\mathrm{erf}(v)\,\mathrm{d}v$$

$$= \frac{b-a}{\sqrt{2\pi}(2k+1)!\, 2^k} \left(\frac{(-1)^k\,(2k)!}{2^{k+1/2}\, k!}\right)$$

$$= (-1)^k\,\frac{(b-a)\,(2k)!}{2^{2k+1}\,\sqrt{\pi}\,(2k+1)!\, k!}$$

Term $I_{2,k}$ is zero for all k except

$$I_{2,0} = \frac{b+a}{2\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-u^2/2}\,\mathrm{d}u = \frac{b+a}{2}$$

It follows that

$$\beta_0 = \frac{a+b}{2}, \quad \beta_{2k} = 0, \text{ and } \beta_{2k+1} = (-1)^k\,\frac{(b-a)\,(2k)!}{2^{2k+1}\,\sqrt{\pi}\,(2k+1)!\, k!}$$

which is consistent with Eq. (14).

C   Lower bound on $\mathrm{E}[h_n(W)^4]$

It follows from the orthogonality properties of Hermite polynomials that (see [2], Eq. (2.3))

$$h_n(x)^2 = \sum_{k=0}^{n} \frac{(n!)^2}{k!\,((n-k)!)^2}\, h_{2(n-k)}(x)$$

for $x \in \mathbb{R}$. Hence, we have

$$\mathrm{E}[h_n(W)^4] = \sum_{k,l=0}^{n} \frac{(n!)^2}{k!\,((n-k)!)^2} \frac{(n!)^2}{l!\,((n-l)!)^2}\, \mathrm{E}[h_{2(n-k)}(W)\, h_{2(n-l)}(W)]$$

$$= \sum_{k=0}^{n} \frac{(n!)^4}{(k!)^2\,((n-k)!)^4}\, (2(n-k))! \qquad (15)$$

where the last line follows from Eq. (4). We note that all summands are non-negative so that any term of Eq. (15) provides a lower bound for $\mathrm{E}[h_n(W)^4]$. For example, the $k=0$ term implies

$$\mathrm{E}[h_n(W)^4] \geq (2n)!,\ \forall n \geq 0, \qquad (16)$$

and this lower bound is sufficient for the proof considered in Example 2. A more stringent lower bound is required for Example 3 and is given by Eq. (15) with $k = (n-1)/2$ assumed an integer, *i.e.*,

$$\mathrm{E}[h_n(W)^4] \geq \frac{(n!)^4\,(n+1)!}{(((n-1)/2)!)^2\,(((n+1)/2)!)^2}$$

or, equivalently

$$\mathrm{E}[h_{2n+1}(W)^4] \geq \frac{((2n+1)!)^4\,(2n+2)!}{(n!)^2\,((n+1)!)^4} = 2\,\frac{(2n+1)^5\,((2n)!)^5}{(n!)^6\,(n+1)^3},\ \forall n \geq 0. \qquad (17)$$

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