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Technical note

Propagation of input model uncertainties with different marginal distributions using a hybrid polynomial chaos expansion

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ABSTRACT

We propose the use of a hybrid polynomial chaos expansion using both Legendre and Hermite polynomials to assess the combined effect of uniform and Gaussian distributed uncertainties. We show that the hybrid method converges exponentially with respect to the polynomial order of the hybrid basis. We also show that mapping the uniformly distributed uncertainties to a Gaussian probability then expanding with a purely Hermite basis results in a severely deteriorated convergence rate.

1. Introduction

In recent years a great deal of research has been dedicated to quantifying the effect that input parameter uncertainties have on the output of a computational model. There are many methods available for solving such problems, see (Cacuci, 2003; Stefanou, 2009) for a review of some, but the technique that we are interested in, which has received considerable attention over the last ten years, is the method of polynomial chaos (Wiener, 1938; Xiu and Karniadakis, 2002; Ghanem, 1999).

The method of polynomial chaos has been applied across many disciplines including fluid flow (Najm, 2009), structural dynamics and neutronic systems (Williams, 2007; Williams, 2010). In the original work by Wiener (Wiener, 1938), the random fluctuation of model parameters (input or output) was represented with an expansion of Hermite polynomials with Gaussian random variables. For any random process, this expansion converges in the L_2 sense to any L_2 functional. In other words, the Hermite expansion converges with increasing polynomial order to any random process with finite variance. However, the optimal (exponential) rate of convergence is only achieved for Gaussian processes. For other non-Gaussian processes, the rate may be substantially reduced. This deterioration in convergence behaviour led to the work by Xiu and Karniadakis (2002) who suggested an optimal description of different distribution types by using a more general framework called Askey chaos. This is also referred to as generalised polynomial chaos (GPC). In this approach the orthogonal polynomial chaos basis is chosen so that the weight function is the same as the probability density function of the random variables representing the uncertainty. In their work (Xiu and Karniadakis, 2002), the authors showed exponential convergence rates for each Askey polynomial for its corresponding stochastic process. They also demonstrated the sub-optimal convergence rates when the optimal Askey polynomial was not employed.

In many engineering applications, including reactor physics and criticality calculations, a situation may arise where the uncertainties associated with input parameters are described with different probability distributions. For example, a reactor lattice pin cell may have nuclear data uncertainties described with a Gaussian distribution whereas the temperature of the fuel and moderator, etc. are described using a uniform distribution. In this note, we extend the work in Xiu and Karniadakis (2002). We propose a combination of the optimal expansions for each probability distribution to form a hybrid polynomial basis. We first show that a tensor product of different Askey polynomials is a basis for the tensor product of their corresponding probability spaces. We then illustrate the theory using a simple numerical example which employs both uniform and Gaussian distributions.

2. Theory

When the inputs to a model have an associated uncertainty, the output(s) are also uncertain. To model this uncertainty, the input uncertainty is represented parametrically by a set of random variables which we denote $\xi = \{\xi_1, \ldots, \xi_M\}$. Here M is the total number of random variables. More generally this may be written as

$$\mathrm{X}(\xi) = \mathcal{L}(\boldsymbol{\alpha}(\xi)) \tag{1}$$

where X is the response parameter, $\boldsymbol{\alpha}(\xi) = \{\alpha_1(\xi), \ldots, \alpha_N(\xi)\}$ is the set of all uncertain input parameters (N being the total number) and $\mathcal{L}$ is a mathematical operator describing the model.

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The mean, variance and higher order statistics of the response parameter can be calculated via integration, namely

$$\mu_X = \int d\xi_1 \ldots \int d\xi_M X(\xi)p(\xi) \tag{2}$$

$$v_X = \int d\xi_1 \ldots \int d\xi_M X^2(\xi)p(\xi) - \mu_X^2 \tag{3}$$

with μ and v representing the mean and variance respectively. The function $p(\xi)$ is the probability density function (PDF) of the random variable ξ. For the case when all variables in the set ξ are independent, the PDF has the form

$$p(\xi) = \prod_{i=1}^{M} p(\xi_i) \tag{4}$$

2.1. Polynomial chaos for mixed uncertainties

The set $\xi(\theta)$, introduced above, is defined on a probability space denoted by $(\Theta, \mathcal{B}, \mu)$ where Θ is the set of all possible outcomes (called the sample space), θ is a random event belonging to Θ and $\mathcal{B}$ is a non-empty collection of subsets of Θ and is called a sigma-field on Θ. The symbol μ is a probability measure on $\mathcal{B}$ and is a function that maps $\mathcal{B}$ onto the real space $[0, 1]$. Let us now denote $L_2(\Theta, \mathcal{B}, \mu)$ as the space of real random variables X with finite second order moments

$$\mathbb{E}[X^2] = \int X(\xi)^2 p(\xi) d\xi < \infty \tag{5}$$

where $\mathbb{E}$ is the mathematical expectation and $p(\xi)$ is the PDF as defined in Eq. (4). Equipped with an inner product

$$< X_1 X_2 >= \mathbb{E}[X_1 X_2] = \int X_1(\xi) X_2(\xi) p(\xi) d\xi \tag{6}$$

this space is a Hilbert space.

If $X(\theta) \in L_2(\Theta, \mathcal{B}, \mu)$ and all ξ are statistically independent then, according to Xiu and Karniadakis (2002), $X(\xi(\theta))$ may be expanded as follows:

$$X(\xi(\theta)) = a_0 I_0 + \sum_{i_1=1}^{\infty} \alpha_{i_1} I_1(\xi_{i_1}(\theta)) + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1} \alpha_{i_1,i_2} I_2(\xi_{i_1}(\theta),\ \xi_{i_2}(\theta)) + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} \alpha_{i_1,i_2,i_3} I_3(\xi_{i_1}(\theta),\ \xi_{i_2}(\theta), \xi_{i_3}(\theta)) + \ldots \tag{7}$$

where $I_n(\xi_{i_1}(\theta), \ldots, \xi_{i_n}(\theta))$ denotes the Wiener–Askey polynomial chaos of order n in terms of the random vector $\xi = \{\xi_{i_1}, \ldots, \xi_{i_n}\}$. For notational convenience, we may write

$$X(\xi) = \sum_{i=1}^{\infty} \alpha_i \Phi_i(\xi) \tag{8}$$

where there is a one-to-one correspondence between the functions $I_n(\xi_{i_1}, \ldots, \xi_{i_n})$ and $\Phi_i(\xi)$.

Consider now a random process Y which belongs to the space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ where $\mathcal{H}_1 = L_2(\Theta_1, \mathcal{B}_1, \mu_1)$ and $\mathcal{H}_2 = L_2(\Theta_2, \mathcal{B}_2, \mu_2)$ are Hilbert spaces. Supposing that $\{\phi_i\}$ and $\{\eta_i\}$ are GPC bases for $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively, then we wish to know if we may expand Y with the following

$$Y = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \alpha_{ij} \phi_i(\xi) \eta_j(\zeta) \tag{9}$$

For $X_1 \in \mathcal{H}_1$ and $X_2 \in \mathcal{H}_2$ we may write

$$X_1(\xi) = \sum_i c_i \phi_i(\xi) \quad X_2(\zeta) = \sum_j d_j \eta_j(\zeta) \tag{10}$$

where ϕ and η are the optimal polynomial bases corresponding to the probability measures μ_1 and μ_2 respectively. We can see straight away that the hybrid basis is orthogonal from the following

$$\langle \phi_1 \otimes \eta_1, \phi_2 \otimes \eta_2 \rangle = \langle \phi_1, \phi_2 \rangle \langle \eta_1, \eta_2 \rangle \tag{11}$$

we also have $\sum_i |c_i|^2 < \infty$ and $\sum_j |d_j|^2 < \infty$. Thus $\sum_{ij} |c_i d_j| < \infty$, and therefore, $\sum_{ij} |c_i d_j| < \infty$. Consequently, we know that $\sum_{i<m,j<n} c_i d_j \phi_i \otimes \eta_j$ converges as $n, m \to \infty$. Therefore,

$$\left\| X_1 \otimes X_2 - \sum_{i<m,j<n} c_i d_j \phi_i \otimes \eta_j \right\| \to 0 \quad \text{as } m, n \to \infty \tag{12}$$

Thus, $\{\phi_i \otimes \eta_j\}$ is a basis for $\mathcal{H}_1 \otimes \mathcal{H}_2$.

The mean and variance of Eq. (9) can now be calculated in the usual way, namely

$$\overline{Y} = \alpha_{00} \tag{13}$$

$$v_Y = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \alpha_{ij} < \phi_i^2 >< \eta_j^2 > \tag{14}$$

3. Numerical example

As an example, we investigate the simple expression for the infinite multiplication factor k_∞:

$$k_\infty(\xi, \zeta) = \frac{v(\xi)\Sigma_f}{\Sigma_a(\zeta)} \tag{15}$$

where v is the average number of neutrons produced per fission and Σ_f and Σ_a are the fission and absorption cross sections respectively. We assume that the absorption cross section and v have an associated uncertainty which we represent parametrically using the random variables ξ and ζ, namely

$$v(\xi) = \bar{v}(1 + R\xi) \quad \xi \in [-\infty : \infty] \tag{16}$$

$$\Sigma_a(\zeta) = \overline{\Sigma_a}\left(1 + \sqrt{3}R\zeta\right) \quad \zeta \in [-1 : 1] \tag{17}$$

The fission cross section is assumed to have no uncertainty. Here R is the relative uncertainty and is defined as

$$R = \frac{\sqrt{v}}{\mu} \tag{18}$$

In Eqs. (16) and (17) we note that the random variables have different supports. With the following probability distributions:

$$p(\xi) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{\xi^2}{2}\right\} \tag{19}$$

$$p(\zeta) = \frac{1}{2} \tag{20}$$

we can see that v is described by a Gaussian distribution and Σ_a by a uniform distribution.

The mean and variance of Eq. (32) using (2) and (3) can be calculated exactly and are given by the following:

$$\mu_{k_\infty} = \int_{-\infty}^{\infty}\int_{-1}^{1} k_\infty(\xi, \zeta) p(\xi) p(\zeta) d\xi d\zeta = -\frac{\bar{v}\Sigma_f}{2\overline{\Sigma_a}R\sqrt{3}} \log\left\{\frac{1-\sqrt{3}R}{1+\sqrt{3}R}\right\} \tag{21}$$

$$v_{k_\infty} = \int_{-\infty}^{\infty}\int_{-1}^{1} k_\infty^2(\xi, \zeta) p(\xi) p(\zeta) d\xi d\zeta - \mu_{k_\infty}^2 = \frac{\bar{v}^2 \overline{\Sigma_f}^2 (1 + R^2)}{\overline{\Sigma_a}(1 - 3R^2)} - \mu_{k_\infty}^2 \tag{22}$$

We must note that solutions to Eqs. (21) and (22) are only available for values of $R \leqslant \frac{1}{\sqrt{3}} \approx 57.7\%$.