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Short communication

On convergence of moments in uncertainty quantification based on direct quadrature

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ABSTRACT

Theoretical results for the convergence of statistical moments in numerical quadrature based polynomial chaos computational uncertainty quantification are presented in this work. This is accomplished by considering the computation of the moments through a direct numerical quadrature method, which is shown to be equivalent to stochastic collocation. For problems which involve output variables which have a polynomial dependence on the random input variables, lower bound expressions are derived for the number of quadrature points required for convergence of arbitrary order moments. In addition, an error expression is derived for when this lower bound is used for problems which have a higher degree of continuity than what was assumed when the bounds are computed. The theoretical results are demonstrated through a simple random algebraic problem and a nonlinear plate problem. The results presented in this work provide further insight into the widely used polynomial chaos expansion method of uncertainty quantification along with presenting simple expressions which can be used for uncertainty quantification code verification.

1. Introduction

The process of uncertainty quantification (UQ) results in a measure of the effect of uncertainty in a system input on the system response quantities of interest. In the design of engineering systems, the information produced from uncertainty quantification can be used as a tool for enabling quantitative risk analysis [1]. When the so-called system involves a computational model, this is accomplished through the propagation of model input uncertainty through the computational model to determine the statistics of the model outputs. These statistics can then be used to determine the probability of undesirable events (outputs) which in turn can be used to give a measure of the risk involved in a given "activity". Several examples of the application of uncertainty quantification for problems (activities) of interest to the engineering community are discussed in Refs. [2–4].

When discussing types of model input uncertainty, the classification provided in Ref. [5] is often used. In this classification three types of uncertainty are recognized: aleatory or irreducible uncertainty; epistemic uncertainty; and uncertainty due to human error. When considering computational uncertainty the first two are relevant [6,7] and relate to a lack of knowledge in the true physics of the problem (epistemic) and randomness in a system (model) parameters (aleatory). Aleatory uncertainty can normally be put in the framework of a probabilistic description while epistemic uncertainty is often difficult to quantify. In this paper we will deal only with aleatory uncertainty.

Computational uncertainty quantification methods can be intrusive or non-intrusive. Most intrusive methods can be thought of as weighted-residual methods whereby the (random) response variables in a differential equation are expanded in a finite series of basis functions (functions of the random input variables) and then the error in the approximation is forced to be orthogonal to a "test" functional space (from considerations of error minimization). This results in a set of deterministic (differential) equations for the coefficients in the expansion. On the other hand in non-intrusive methods, deterministic simulation tools can be treated as "black boxes" and hence simulation code modification is not required. A typical non-intrusive uncertainty quantification scheme consists of, similar to intrusive methods, expanding the random response variable in a finite series of basis functions whose coefficients are then computed by sampling the black box simulation and then using spectral projection or linear regression [8]. For either method, intrusive or non-intrusive, once the coefficients in the expansion are found they can be used to reconstruct the response which then can be used to determine statistical quantities of interest.

The most common functional spaces used in the expansions correspond to what is called generalized polynomial chaos [9–14] and can be generated using the Wiener–Askey scheme. The first

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instance of this was introduced by Wiener [15] as the span of the Hermite polynomial functionals of a Gaussian random process and is often called Wiener's polynomial chaos or Homogeneous chaos. Depending on the type of continuous random variable, the Wiener–Askey scheme generates polynomials which are orthogonal to the measure of the random variable.

When using uncertainty quantification analysis for an engineering system, an important objective should be the determination of a set of design criteria which can be used in a probabilistic context so that a reliability analysis is permitted [16–18]. In this context, the statistical moments (including mean, variance, skewness, kurtosis) of the system response can provide bounds about its expected range along with giving meaningful information about the reliability of the system with random inputs. The moments can also be used together with some expansion, such as the Edgeworth expansion [19], to approximate the probability distribution function of the response process. In order for the uncertainty quantification analysis to provide useful information about system reliability, the moments of interest should be estimated accurately to within a user-defined tolerance. Some key questions which should then be asked are: (a) *what smart choices can the analyst make in an a priori sense to ensure that moments up to a desired order are estimated accurately?* and (b) *how many samples are necessary for accurate uncertainty quantification, including asymptotic convergence in (point estimates of) the probability density of the system output and convergence in moments up to an arbitrarily high order?* In other words (regarding question (a)), if something is known about the functional dependence of the random response on the random input, can the minimum number of samples in a non-intrusive uncertainty quantification analysis be chosen ahead of time such that all moments up to a given order are guaranteed to be converged? It appears that convergence in probability density functions of system outputs (regarding question (b)) is dependent on the type of reconstruction approach used (e.g. Edgeworth series, Maximum Entropy approach) to determine the probability density function based on the underlying moments (up to a known order).

In this paper we will present analysis which addresses question (a). Specifically, we will provide theoretical results on the necessary conditions for the number of samples needed in a non-intrusive polynomial chaos expansion (PCE) to provide statistical moments of a response variable within a given error bound. For random response variables which are given in terms of polynomials of the random input variables, these conditions provide a lower bound on the number of samples needed for an exact evaluation of the statistical moments. In addition an expression is developed for the error incurred if this lower bound is used for a problem which has a higher degree of continuity than which was assumed when the bound was computed. In order to produce these results, we will develop the non-intrusive uncertainty quantification process directly in terms of numerical quadrature of the statistical moments [20], the result of which will be shown to be equivalent to stochastic collocation [8]. In addition to aiding in the development of the theoretical results, the authors feel that presenting the computation of statistical moments from a direct quadrature perspective presents a simple, straightforward way of introducing the topic. The theoretical results on the number of samples needed for statistical moment convergence will be demonstrated using a simple numerical example. It may be noted that in our analysis (regarding determination of minimum number of samples needed for convergence of moments up to a desired order), we assume that the exact functional dependence of the system response on the system input is known and can be represented via polynomials. Although this may not often be the case, the present analysis serves as an important tool for code verification and validation. As this work is particularly focused on identifying the conditions for accurate estimation of moments (of arbitrary order) using quadrature, it could complement many methods in reliability analysis that involve moment dependent (e.g. variance based) or moment independent (e.g. entire output distribution) uncertainty measures [17,18,13,14].

2. Theory

In this section we will present the salient theoretical details which are needed to derive the theoretical results for the PCE method. Further details on the generalized PCE can be found, for example, in Refs [3,10].

2.1. A direct quadrature view of the computation of moments of random response

The nth moment of a random variable u which is a function of N independent random variables, denoted here as $\boldsymbol{\xi}(\theta)=\{\xi_1(\theta), \xi_2(\theta),\ldots,\xi_N(\theta)\}$, is given by the expression

$$\langle u^n(\boldsymbol{\xi})\rangle = \int_{\Omega} u(\boldsymbol{\xi}(\theta))^n p(\boldsymbol{\xi}(\theta))\, d\boldsymbol{\xi}(\theta), \tag{1}$$

where θ is a random event and Ω and $p(\boldsymbol{\xi}(\theta))$ denote the support and probability density (respectively) corresponding to $\boldsymbol{\xi}$.

The basis of the direct quadrature computation is to use numerical (Gauss) quadrature to compute the integral in Eq. (1). Using Gauss quadrature a one-dimensional integral of the form

$$\int_a^b f(x)w(x)\, dx \tag{2}$$

is approximated with the M-point quadrature formula given by

$$\int_a^b f(x)w(x)\, dx \approx \sum_{i=1}^{M} f(x_i)\tilde{w}_i. \tag{3}$$

The evaluation point x_i corresponds to the ith root of the orthogonal polynomials with the weighting function $w(x)$. Common weighting functions (with the corresponding support) include 1 (Gauss–Legendre), $1/(\sqrt{1-x^2})$ (Gauss–Chebyshev) and e^{-x^2} (Gauss–Hermite). Higher dimensional integrals can be computed using tensor products of one-dimensional formulas or, if the dimension is large, a sparse grid technique such as Smolyak quadrature [21]. If $f(x)$ is continuous on $[a,b]$, then it can be shown [22] that the approximations in Eq. (3) converge to the integral as $M\to\infty$.

For a function $f(x)\in C^{2M}[a,b]$ the error in Eq. (3) is given by

$$E=\frac{f^{2M}(\zeta)}{(2M)!}\langle \Phi_M,\Phi_M\rangle, \tag{4}$$

where $f^{2M}(\zeta)$ corresponds to the $2M$ th derivative of f and $a<\zeta<b$. Also $\langle \Phi_M,\Phi_M\rangle$ corresponds to the inner product of the Mth-order polynomial which is orthogonal to the weighting function $w(x)$ in Eq. (3). From Eq. (4) it can be shown that M point Gauss quadrature is exact for a polynomial of degree at most $2M-1$.

For clarity of presentation we will now restrict ourself to $N=1$, i.e. a one-dimensional space of a single random variable (ξ). Additional consideration of results for higher dimensions will be given where necessary. For one dimension, Eq. (1) can now be approximated using numerical quadrature as

$$\begin{aligned}\langle u^n(\xi)\rangle &= \int_a^b u(\xi(\theta))^n p(\xi(\theta))\, d\xi(\theta)\\ &\approx \sum_{i=1}^{M} u(\xi_i)^n \tilde{w}_i,\end{aligned} \tag{5}$$