Reliability Engineering and System Safety 96 (2011) 1092–1113

Contents lists available at ScienceDirect

Reliability Engineering and System Safety

journal homepage: www.elsevier.com/locate/ress

Mixed aleatory-epistemic uncertainty quantification with stochastic expansions and optimization-based interval estimation

M.S. Eldred [a,*], L.P. Swiler [a], G. Tang [b]

[a] Optimization and Uncertainty Quantification Department, Sandia National Laboratories, P.O. Box 5800, Albuquerque, NM 87185-1318, United States[1]
[b] Department of Aeronautics and Astronautics, Stanford University, Stanford, CA 94305, United States

ARTICLE INFO

Article history:
Received 24 March 2010
Received in revised form
17 November 2010
Accepted 20 November 2010
Available online 7 April 2011

Keywords:
Uncertainty quantification
Epistemic
Aleatory
Polynomial chaos expansion
Stochastic collocation
Interval optimization
Second-order probability
Dempster–Shafer evidence theory

ABSTRACT

Uncertainty quantification (UQ) is the process of determining the effect of input uncertainties on response metrics of interest. These input uncertainties may be characterized as either aleatory uncertainties, which are irreducible variabilities inherent in nature, or epistemic uncertainties, which are reducible uncertainties resulting from a lack of knowledge. When both aleatory and epistemic uncertainties are mixed, it is desirable to maintain a segregation between aleatory and epistemic sources such that it is easy to separate and identify their contributions to the total uncertainty. Current production analyses for mixed UQ employ the use of nested sampling, where each sample taken from epistemic distributions at the outer loop results in an inner loop sampling over the aleatory probability distributions. This paper demonstrates new algorithmic capabilities for mixed UQ in which the analysis procedures are more closely tailored to the requirements of aleatory and epistemic propagation. Through the combination of stochastic expansions for computing statistics and interval optimization for computing bounds, interval-valued probability, second-order probability, and Dempster–Shafer evidence theory approaches to mixed UQ are shown to be more accurate and efficient than previously achievable.

1. Introduction

Uncertainty quantification (UQ) is the process of determining the effect of input uncertainties on response metrics of interest. These input uncertainties may be characterized as either aleatory uncertainties, which are irreducible variabilities inherent in nature, or epistemic uncertainties, which are reducible uncertainties resulting from a lack of knowledge. Since sufficient data is available for characterizing aleatory uncertainties, probabilistic methods are commonly used for computing response distribution statistics based on input probability distribution specifications. Conversely, for epistemic uncertainties, data is generally too sparse to support objective probabilistic input descriptions, leading either to subjective probabilistic descriptions (e.g., assumed priors in Bayesian analysis) or nonprobabilistic methods based on interval specifications.

1.1. Probabilistic UQ for aleatory uncertainties

One technique for the analysis of aleatory uncertainties using probabilistic methods is the polynomial chaos expansion (PCE) approach to UQ. For smooth functions (i.e., analytic, infinitely differentiable) in L^2 (i.e., possessing finite variance), exponential convergence rates can be obtained under order refinement for integrated statistical quantities of interest such as mean, variance, and probability. In this work, generalized polynomial chaos using the Wiener-Askey scheme [1] provides a foundation in which Hermite, Legendre, Laguerre, Jacobi, and generalized Laguerre orthogonal polynomials are used for modeling the effect of continuous uncertain variables described by normal, uniform, exponential, beta, and gamma probability distributions, respectively.[2] These polynomial selections are optimal for these distribution types since they are orthogonal with respect to an inner product weighting function that corresponds[3] to the probability density functions for these continuous distributions. Orthogonal polynomials can be computed for any positive weight function, so these five classical orthogonal polynomials may be augmented with numerically generated polynomials for other probability

* Corresponding author.
E-mail addresses: mseldre@sandia.gov (M.S. Eldred), lpswile@sandia.gov (L.P. Swiler), garytang@stanford.edu (G. Tang).
URL: http://www.cs.sandia.gov/~mseldre (M.S. Eldred).

[1] Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

[2] Orthogonal polynomial selections also exist for discrete probability distributions, but are not explored here.

[3] Identical support range; weight differs by at most a constant factor.

0951-8320/$ - see front matter © 2011 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ress.2010.11.010

distributions (e.g., for lognormal, extreme value, and histogram distributions). When independent standard random variables are used (or computed through transformation), the variable expansions are uncoupled, allowing the polynomial orthogonality properties to be applied on a per-dimension basis. This allows one to mix and match the polynomial basis used for each variable without interference with the spectral projection scheme for the response.

In non-intrusive PCE, simulations are used as black boxes and the calculation of chaos expansion coefficients for response metrics of interest is based on a set of simulation response evaluations. To calculate these response PCE coefficients, two primary classes of approaches have been proposed: spectral projection and linear regression. The spectral projection approach projects the response against each basis function using inner products and employs the polynomial orthogonality properties to extract each coefficient. Each inner product involves a multi-dimensional integral over the support range of the weighting function, which can be evaluated numerically using sampling, tensor-product quadrature, Smolyak sparse grid [2], or cubature [3] approaches. The linear regression approach uses a single linear least squares solution to solve for the set of PCE coefficients which best match a set of response values obtained from either a design of computer experiments ("point collocation" [4]) or from the subset of tensor Gauss points with highest product weight ("probabilistic collocation" [5]).

Stochastic collocation [6] (SC) is a second stochastic expansion approach that is closely related to PCE. As for PCE, exponential convergence rates can be obtained under order refinement for integrated statistical quantities of interest, provided that the response functions are smooth with finite variance. The primary distinction is that, whereas PCE estimates coefficients for known orthogonal polynomial basis functions, SC forms Lagrange interpolation functions for known coefficients. Interpolation is performed on structured grids such as tensor-product or sparse grids. Starting from a tensor-product multidimensional Lagrange interpolant, we have the feature that the ith interpolation polynomial is 1 at collocation point i and 0 for all other collocation points, leading to the use of expansion coefficients that are just the response values at each of the collocation points. Sparse interpolants are weighted sums of these tensor interpolants; however, they are only interpolatory for sparse grids based on fully nested rules and will exhibit some interpolation error at the collocation points for sparse grids based on non-nested rules. A key to maximizing performance with SC is performing collocation using the Gauss points and weights from the same optimal orthogonal polynomials used in PCE. For use of standard Gauss integration rules (not nested variants such as Gauss–Patterson or Genz–Keister) within tensor-product quadrature, tensor PCE expansions and tensor SC interpolants are equivalent in that identical polynomial approximations are generated [7]. Moreover, this equivalence can be extended to sparse grids based on standard Gauss rules, provided that a sparse PCE is formed based on a weighted sum of tensor expansions [8].

Once PCE or SC representations have been obtained for a response metric of interest, analytic expressions can be derived for the moments of the expansion (from integration over the aleatory/probabilistic random variables) as well as for various sensitivity measures. Local sensitivities (i.e., derivatives) and global sensitivities [9] (i.e., ANOVA, variance-based decomposition) of the response metrics may be computed with respect to the expansion variables, and local sensitivities of probabilistic response moments may be computed with respect to other nonprobabilistic variables [10] (i.e., design or epistemic uncertain variables). This latter capability allows for efficient design under uncertainty and mixed aleatory-epistemic UQ formulations involving moment control or bounding. This paper presents two approaches for calculation of sensitivities of moments with respect to nonprobabilistic dimensions (design or epistemic), one involving response function expansions over both probabilistic and nonprobabilistic variables and one involving response derivative expansions over only the probabilistic variables.

1.2. Mixed aleatory-epistemic UQ

A common approach to quantifying the effects of mixed aleatory and epistemic uncertainties is to separate the aleatory and epistemic variables and perform nested iteration. This separation allows the use of strong probabilistic inferences where possible, while employing alternative inferences only where necessary. Traditionally, this has involved a nested sampling approach, in which each sample drawn from the epistemic variables on the outer loop results in a sampling over the aleatory variables on the inner loop. In this fashion, we generate families or ensembles of response distributions, where each distribution represents the uncertainty generated by sampling over the aleatory variables. Plotting an entire ensemble of cumulative distribution functions (CDFs) in a "horsetail" plot allows one to visualize the upper and lower bounds on the family of distributions (see Fig. 1). However, nested iteration can be computationally expensive when it is implemented using two random sampling loops. Consequently, when employing simulation-based models, the nested sampling must often be under-resolved, particularly at the epistemic outer loop, resulting in an under-prediction of credible output ranges. Thus, the central goal in this work is to preserve the advantages of uncertainty separation (visualization, interpretation, and tailoring of inferences), but address issues with accuracy and efficiency within the nested iteration by closely tailoring the algorithmic approaches to the propagation needs at each level.

We propose a new approach for performing mixed UQ in which the inner-loop CDFs will be calculated using a stochastic expansion method (using either aleatory expansions formed for each instance of the epistemic variables or combined expansions over both variable sets), and outer loop bounds can be computed with optimization-based interval estimation (using either local gradient-based or global nongradient-based optimizers). The advantages of this approach can be significant, due to several factors. First, the stochastic expansion methods can be much more efficient than sampling for calculation of moments or CDF

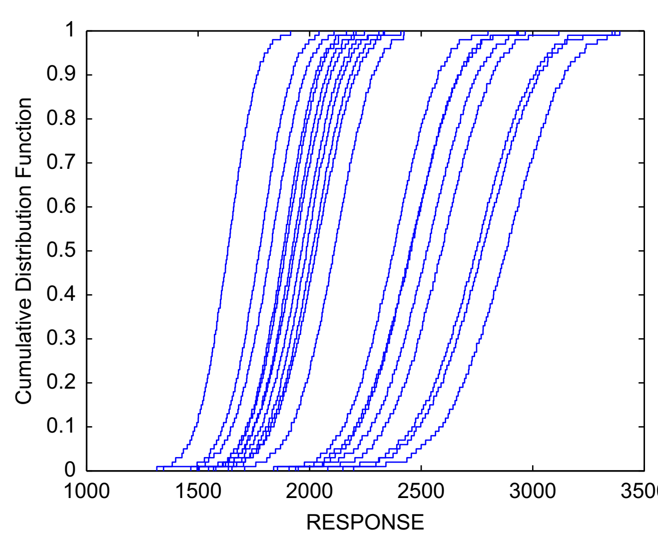

Fig. 1. Example CDF ensemble. Commonly referred to as a "horsetail" plot.