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Procedia Social and Behavioral Sciences 2 (2010) 7765–7767

Procedia Social and Behavioral Sciences

Sixth International Conference on Sensitivity Analysis of Model Output

Sensitivity analysis using stochastic expansion methods to calculate variance-based sensitivity indices

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Abstract

Sensitivity analysis and uncertainty quantification are computationally expensive procedures. Stochastic expansion methods are an alternative approach for performing SA and UQ, and usually require fewer function evaluations. Recent work has extended non-intrusive stochastic expansion methods for calculating sensitivity indices. We examine the application of these techniques to a case in which data are generated from coupled, nonlinear partial differential equations. The values we analyze are generated from the numerical solution of the PDEs, in which we systematically vary both (i) fundamental modeling parameters and (ii) the underlying numerical algorithms. Our goal is to compare the performance of the sensitivity index calculations using sampling based methods and stochastic expansion methods, to gain an understanding of the strengths and weaknesses of both approaches.

Keywords: Conservation laws, compressible flow, sensitivity analysis, uncertainty quantification, stochastic expansion

1. Main text

Sensitivity analysis (SA) and uncertainty quantification (UQ) are critical capabilities used to understand the behavior of large-scale computer simulations. As part of understanding model behavior, one might want to identify the most significant factors or input variables affecting the model predictions or results (sensitivity analysis). Another common goal is to characterize the distribution of output measures based on uncertain inputs (uncertainty quantification). A wide variety of methods exists for performing SA and UQ; see, e.g., Helton et al. (2006), Saltelli et al. (2000), Iman and Helton (1988), and Storlie and Helton (2008). Many of these methods rely on sampling the input distributions. Sampling-based methods can be very expensive, requiring many evaluations of the simulation. Often the computational cost of performing one simulation run is expensive and the cost of running an ensemble of runs becomes prohibitively large. In these situations, UQ and SA is either not performed or may be under-resolved.

Stochastic expansion methods produce functional representations of stochastic variability, where model output is represented by analytic functions of stochastic inputs, as described by Eldred (2009) and Eldred et al. (2008). One

doi:10.1016/j.sbspro.2010.05.218

stochastic expansion method, the Polynomial Chaos Expansion (PCE), represents the output as a sum of orthogonal polynomial basis functions, where these polynomials are chosen based on the input distribution type. Once the coefficients of the orthogonal polynomials are determined, one has an analytic formulation of the output from which moments can be easily calculated and the expansion can be sampled extensively to get accurate cumulative distribution function estimates. The popularity of stochastic expansion methods as applied in a "non-intrusive, black-box" mode has increased significantly in the past decade. In large part, this popularity is due to the ability of stochastic expansion methods to accurately quantify system uncertainty with fewer function evaluations than traditional sampling. Recently, Sudret (2008) and Tang et al. (2009) extended the stochastic expansion methods so that these expansions are used directly to calculate variance-based sensitivity indices. This approach is very efficient: the calculation of input sensitivities does not require additional function evaluations beyond those needed to construct the stochastic expansion. The sensitivity indices are analytic functions of the stochastic expansion.

In this study, we apply formulations of variance-based sensitivity indices (also called Sobol' indices) based on two classes of stochastic expansion methods: polynomial chaos expansions (PCE) and stochastic collocation (SC) methods. These methods are applied to a set of coupled, nonlinear partial differential equations (PDEs) that govern compressible flow problem of Sod (1978). We examine the sensitivity of the computed solution output to the structural parameters involved in determining the equations, and to the parameters associated with the algorithms used to integrate the equations. This work is a companion to that described in the abstract by Kamm et al. for this SAMO conference that examines the same problem but uses sampling methods and other SA approaches. The goal of having both papers focus on the same application problem is to understand the pros and cons of the various methods. For example, the stochastic expansion methods tend to work very well with small numbers of uncertain variables but suffer from the "curse of dimensionality" as the number of inputs increases, for cases where the expansion is based on tensor product quadrature. There are methods that can help overcome this issue, such as adaptive sampling and sparse grids. Also, the stochastic expansion methods cannot currently treat discrete variables; this is an area of active research. We are simply examining how stochastic expansion methods work and characterizing when they perform well in terms of calculating sensitivity indices.

Our approach will be to perform tensor product quadrature together with sparse grid and LHS sampling to generate the points in the input space at which the simulation will be evaluated. The shock physics simulations will be performed in ALEGRA (Robinson (2008)). Then, the stochastic expansions will be constructed and used to calculate the sensitivity indices. The software framework we will use is the DAKOTA toolkit (see www.cs.sandia.gov/DAKOTA). We expect this work will highlight some of the benefits and disadvantages of the stochastic expansion methods used in variance-based approaches. We anticipate that this work will be a useful guide and benchmark for more complex simulation exercises.

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