Commun. Comput. Phys.
doi: 10.4208/cicp.230909.160310s

Vol. **9**, No. 3, pp. 542-567
March 2011

Variance-Based Global Sensitivity Analysis via Sparse-Grid Interpolation and Cubature

Gregery T. Buzzard and Dongbin Xiu*

Department of Mathematics, Purdue University, West Lafayette, IN 47907, USA.

Received 23 September 2009; Accepted (in revised version) 16 March 2010

Available online 17 September 2010

To the memory of David Gottlieb

Abstract. The stochastic collocation method using sparse grids has become a popular choice for performing stochastic computations in high dimensional (random) parameter space. In addition to providing highly accurate stochastic solutions, the sparse grid collocation results naturally contain sensitivity information with respect to the input random parameters. In this paper, we use the sparse grid interpolation and cubature methods of Smolyak together with combinatorial analysis to give a computationally efficient method for computing the global sensitivity values of Sobol'. This method allows for approximation of all *main effect* and *total effect* values from evaluation of f on a single set of sparse grids. We discuss convergence of this method, apply it to several test cases and compare to existing methods. As a result which may be of independent interest, we recover an explicit formula for evaluating a Lagrange basis interpolating polynomial associated with the Chebyshev extrema. This allows one to manipulate the sparse grid collocation results in a highly efficient manner.

AMS subject classifications: 41A10, 41A05, 41A63, 41A55

Key words: Stochastic collocation, sparse grids, sensitivity analysis, Smolyak, Sobol'.

1 Introduction

The growing popularity of computational models in various fields of science and engineering has led to a corresponding growth in interest in methods to understand parameter spaces. A common task in developing a model is to find parameters $p=(p_1,\cdots,p_n)$ to minimize some cost function, $C(p)$, often a sum of squared differences between model output and experimental data. This is a particularly difficult task when the dimensionality of the parameter space is large and the dependence of C on p is nonlinear. Hence, the development of efficient tools for reducing the size of the search space is vital.

*Corresponding author. *Email addresses:* `buzzard@math.purdue.edu` (G. T. Buzzard), `dxiu@math.purdue.edu` (D. Xiu)

 ©2011 Global-Science Press

Local sensitivity analysis, which computes partial derivatives $\partial C/\partial p_j$, may be used to determine which parameters are relatively more important than others at a single point in the parameter space. In contrast, global sensitivity analysis (GSA) seeks a measure of relative importance over the entire parameter space. One approach to GSA is variance based. With an appropriate measure, we may regard the parameter space as a probability space and C as a random variable on this space. The sensitivity of C to a given parameter p_j is then

$$\frac{\mathrm{Var}_{p_j}\big(E[C|p_j]\big)}{\mathrm{Var}(C)},$$

where $E[C|p_j]$ is the expected value obtained by fixing a given value of p_j and integrating over the remaining variables, and Var_{p_j} is the variance as a function of p_j only. As noted by Saltelli et al. (see [6] and the references therein), this quantity has appeared in various formulations in many places in the literature.

Sobol′ [10] provides a particularly appealing formulation of this quantity as a special case of a more general approach to GSA for arbitrary subsets of parameters. The measure above, which is meant to capture the effect of the single parameter p_j, is often called the *main effect* due to p_j. By considering other subsets containing p_j, the sensitivity values of Sobol′ can be used to identify interaction effects among multiple variables. For instance, by considering the sum of all sensitivity values in which p_j takes part, we obtain what is often called the *total effect* due to p_j. Sobol′ [10] describes a method for evaluating the main effect values using Monte Carlo or quasi-Monte Carlo methods. Saltelli et al. [6] give a Fourier analysis based method for computing both the main and total effects. This is often called the Extended FAST method.

The problem we address in this paper is to use the values of a function computed at the nodes of sparse grids to compute these sensitivity values efficiently. In practice, these function values are obtained through an expensive computation such as solving a large ODE system or a PDE, and these values are often used to construct an interpolating polynomial that approximates the function itself. Here we use both interpolation and cubature with these values to obtain all the main effect and total effect values without further simulation effort. To this end, we demonstrate that even though multi-dimensional Lagrange interpolation polynomials are not easy to manipulate in general, a highly efficient sensitivity analysis based on the Sobol′ decomposition can be accomplished by utilizing the properties of sparse grids and Chebyshev polynomials. Moreover, the algorithm presented here retains the high order approximation accuracy from the sparse-grid simulations and can be carried out completely offline.

For a detailed discussion of many approaches to sensitivity analysis as well as a discussion of the Extended FAST method and many additional references, see [8]. For other approaches to improve the efficiency of computing sensitivity values, see [2,4,7,11] and references therein. In contrast to these methods, our method is based on the idea of stochastic collocation (see, e.g., [16]), which has become popular since [16] introduced the use of sparse grids in the stochastic collocation method. The use of sparse grids alleviates