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Sensitivity analysis techniques applied to a system of hyperbolic conservation laws

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ABSTRACT

Sensitivity analysis is comprised of techniques to quantify the effects of the input variables on a set of outputs. In particular, sensitivity indices can be used to infer which input parameters most significantly affect the results of a computational model. With continually increasing computing power, sensitivity analysis has become an important technique by which to understand the behavior of large-scale computer simulations. Many sensitivity analysis methods rely on sampling from distributions of the inputs. Such sampling-based methods can be computationally expensive, requiring many evaluations of the simulation; in this case, the Sobol' method provides an easy and accurate way to compute variance-based measures, provided a sufficient number of model evaluations are available. As an alternative, meta-modeling approaches have been devised to approximate the response surface and estimate various measures of sensitivity. In this work, we consider a variety of sensitivity analysis methods, including different sampling strategies, different meta-models, and different ways of evaluating variance-based sensitivity indices. The problem we consider is the 1-D Riemann problem. By a careful choice of inputs, discontinuous solutions are obtained, leading to discontinuous response surfaces; such surfaces can be particularly problematic for meta-modeling approaches. The goal of this study is to compare the estimated sensitivity indices with exact values and to evaluate the convergence of these estimates with increasing samples sizes and under an increasing number of meta-model evaluations.

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1. Introduction

Sensitivity analysis is a broad field, with many methods used for many different applications. Here we consider variance-based sensitivity indices developed by Sobol' [1,2], which express relative sensitivities as the fraction of the variance of a model output that can be attributed to each uncertain input. These indices are used, for example, to identify the most influential inputs; with this information, limited resources can be focused on reducing the uncertainty of the most influential inputs so the variance of the outputs can be reduced by the greatest amount. Another use is to identify unimportant inputs to fix (hold constant) in a subsequent uncertainty quantification effort; fixing unimportant inputs reduces the size and complexity of the uncertainty quantification problem.

In this paper we examine several sensitivity analysis approaches. We consider Latin hypercube sampling (LHS) and Sobol' sequences (a type of quasi-Monte Carlo (QMC) sequence) for sampling the input hypercube. We consider two approaches to meta-modeling, which aims to reduce the number of computationally expensive function evaluations, including several state-of-the-art regression based meta-models and non-intrusive polynomial chaos expansion (PCE), a stochastic expansion method. Section 2 describes these techniques and the computation of variance-based sensitivity indices.

In Section 3 we apply these techniques to a canonical shock physics problem. The key features of such problems are that the solutions to the governing equations are often discontinuous, even when the initial conditions are smooth; the character of the governing nonlinear partial differential equations is hyperbolic, with waves propagating in various directions at finite speeds and interacting with other waves; and most solutions are time-dependent. Numerical simulations provide approximate solutions to the governing equations. The numerical solutions, in turn, provide the outputs (responses) for the sensitivity analysis, so our

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simulation code is referred to as the *simulation model*. Particular care was taken so that some outputs are discontinuous functions of the inputs, reflecting the properties of the underlying physics. An exact solution to the governing equations is also known for this shock physics problem, and provides the *exact model*, which can be used to generate alternative output values for the sensitivity analysis.

This shock physics problem is very familiar to those in the field, and a working knowledge of the sensitivities of the problem is generally known. Consequently, this problem was chosen as a test problem on which the various sensitivity analysis techniques could be tested. Since simulations of our test problem are not costly, an exact solution to the sensitivity analysis itself can be obtained by full factorial sampling. This provides an unambiguous metric against which the sensitivity analysis techniques can be compared. Our initial results are presented in Section 4. Our ultimate goal, in the context of discontinuous responses, is to examine the performance of the sensitivity analysis techniques in a rigorous fashion. We hope to determine, for example, the accuracy of the Sobol' indices as a function of the sample size; the accuracy as a function of the PCE order; the accuracy as a function of the number of samples to build a particular meta-model; and what, if anything, can be learned about the response function when various meta-models yield different results.

2. Sensitivity analysis

For a given model with a number of inputs and outputs, sensitivity analysis identifies the inputs that have the greatest influence on each output. In global SA methods including those considered here, this is achieved by repeatedly sampling input values from their distributions, evaluating the model with these values, and measuring the outputs.

2.1. Sobol' sensitivity indices

The sensitivity of an output Y to each input X_i can be quantified by Sobol' sensitivity indices [3]. Traditional regression coefficients only detect linearity or monotonicity, while the variance-based Sobol' indices are not limited in this way. Recall that for a random variable y with probability distribution $p(y)$

$$E(Y) = \int yp(y) dy \quad (1)$$

is the expected value of Y ,

$$E(Y|X_i) = \int yp(y|X_i) dy \quad (2)$$

is the expected value of Y conditioned on X_i , and

$$\text{Var}(Y) = E((Y - E(Y))^2) \quad (3)$$

is the variance of Y . The first-order ("main effects") indices are defined by

$$S_i = \frac{\text{Var}(E(Y|X_i))}{\text{Var}(Y)}. \quad (4)$$

The first-order indices quantify the variability in Y that can be attributed to X_i alone. The total effects indices are defined by

$$T_i = \frac{E(\text{Var}(Y|X_{-i}))}{\text{Var}(Y)}, \quad (5)$$

where $\text{Var}(Y|X_{-i})$ is the variance of Y conditioned on all the inputs except X_i , and quantify the variability in Y that can be attributed to X_i and all of its interactions with other inputs. These indices involve multidimensional integrals that, in practice, are evaluated

approximately. A number of evaluation methods will be described in following sections.

2.2. Sampling

We compute the indices by numerical quadrature when using full-factorial sampling (FFS, which requires the most simulations but gives the best estimates), by two different estimation approaches for smaller sample sizes [4], and by an analytic formula when stochastic expansions are used (described below). In FFS, each input can assume a number of values and the set of samples includes all possible combinations of all input values. Reduced sample sizes are obtained by Latin hypercube sampling [5,6] and quasi-Monte Carlo sequences, which seek to represent the possible input combinations in some balanced fashion.

A good review of QMC sequences is offered by Bratley, Fox, and Niederreiter [7], which includes sequences suggested by Faure, Niederreiter, Halton, Hammersley, Sobol', and other investigators. Such sequences are specifically designed to generate multidimensional samples as uniformly as possible. Unlike random numbers, successive quasi-random points *know* about the position of previously sampled points and fill the gaps between them. For this reason they are also called quasi-random numbers, although they are, in fact, not random at all. In the present work we limit ourselves to an updated version of the Sobol' QMC sequence [8,9], which is characterized by low discrepancy properties (sequence #8192 by Kucherenko [10]). A former version (sequence #51) with good performance is available for free on the JRC web-page [11]. Sobol' sequences outperform crude Monte Carlo sampling in the estimation of multi-dimensional integrals [12].

2.3. Meta-models

From a limited number of costly numerical simulations, a meta-model approximating the response can be developed as an inexpensive alternative. We consider three non-parametric regression methods for meta-modeling. Two of them are based on splines, namely the Adaptive Component Selection and Smoothing Operator (ACOSSO) [13] and the State-Dependent Parameter Regression (SDP) approach [14], and the third is based on kriging (as implemented in the DACE toolbox for MATLAB [15]). We also include a stochastic expansion approach.

The classical approach to smoothing spline ANOVA models is along the lines of Wahba [16] and Gu [17]. Recently, Storlie et al. [13] presented ACOSSO, "a new regularization method for simultaneous model fitting and variable selection in nonparametric regression models in the framework of smoothing spline ANOVA." This method is a multivariate smoothing-spline approach augmented by a weighted, scaled penalty function. It is an improvement of COSSO [18], penalizing the sum of component norms, instead of the squared norm employed in the traditional smoothing spline method.

In a stream of research parallel to multivariate ANOVA smoothing splines, using the so-called State-Dependent Parameter Regression (SDP) approach of Young [19], Ratto et al. [14] developed a non-parametric approach. (This particular type of SDP is often abbreviated as SDR.) It is very similar to smoothing splines and kernel regression methods, based on recursive filtering and smoothing estimation (the Kalman Filter combined with Fixed Interval Smoothing). Such a recursive least-squares implementation has some key characteristics: (a) smoothing hyper-parameters are determined by optimal Maximum Likelihood estimation, allowing an objective estimation of these parameters, and (b) it provides greater flexibility in adapting to local discontinuities, heavy non-linearity and heteroscedastic error terms.

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