

**Sensitivity Analysis Techniques Applied  
to a Model Shock Problem (U)**

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Sensitivity analysis is comprised of techniques to quantify the effect of the input variables on a set of outputs. In particular, such 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 the input distributions. 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 shock-tube problem. By the proper choice of inputs, discontinuous solutions are obtained, thereby 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. (UNC)

## 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. This is achieved by evaluating the model many times using different input values sampled from their distributions and measuring the outputs.

The sensitivity of an output  $Y$  to each input  $X_i$  is quantified by Sobol' sensitivity indices. [5] Traditional regression coefficients only detect linearity or monotonicity, while the variance-based Sobol' indices are not limited in this way. The first-order ("main effects") indices quantify the variability in  $Y$  that can be attributed to  $X_i$  alone, and are defined by

$$S_i = \frac{\text{Var}(E(Y|X_i))}{\text{Var}(Y)}, \quad (1)$$

where  $\text{Var}(\cdot)$  is the variance,  $E(\cdot)$  is the expected value, and  $E(Y|X_i)$  is the expected value of  $Y$  conditioned on  $X_i$ . The total effects indices are defined by

$$T_i = \frac{E(\text{Var}(Y|X_{-i}))}{\text{Var}(Y)}, \quad (2)$$

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 are multidimensional integrals that, in practice, are evaluated approximately. 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 sets of samples [6, 7] as described below, and by an analytic formula when stochastic expansions are used, also 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 sets of samples are obtained by

Latin Hypercube Sampling (LHS) and quasi-Monte Carlo sequences (QMCS), which represent the possible input combinations in a balanced fashion.

We describe sensitivity index estimators from two references, Saltelli et al. [6] and an updated and improved approach from the same group [7]. Each reference provides an estimator for the main effects,  $S_i$ , and total effects,  $T_i$ . Some notation: if we denote the original sample matrices as  $\mathbf{A}$  and  $\mathbf{B}$ , we denote by  $\mathbf{A}_{\mathbf{B}}^{(i)}$  the matrix  $\mathbf{A}$  except for the  $i$ th column, which has been taken from matrix  $\mathbf{B}$ . Similarly,  $\mathbf{B}_{\mathbf{A}}^{(i)}$  is the matrix  $\mathbf{B}$  except for the  $i$ th column, which has been taken from matrix  $\mathbf{A}$ . We define  $\mathbf{C}$  as the matrix with  $2n$  rows and  $d$  columns obtained by appending  $\mathbf{B}$  to  $\mathbf{A}$ .  $\mathbf{C}$  is used in some formulas to estimate the total variance, as all rows of  $\mathbf{C}$  are independent. The mean value is denoted by  $\langle \cdot \rangle$ .

With this notation, given an output function  $f$ , the earlier estimators [6] are computed as follows:

$$S_i = \frac{\frac{1}{n} \sum_{j=1}^n f(\mathbf{A})_j f(\mathbf{B}_{\mathbf{A}}^{(i)})_j - \langle f(\mathbf{A}) \rangle \langle f(\mathbf{B}) \rangle}{\frac{1}{n} \sum_{j=1}^n f(\mathbf{A})_j f(\mathbf{A})_j - \langle f(\mathbf{A}) \rangle \langle f(\mathbf{B}) \rangle}, \quad (3)$$

$$T_i = 1 - \frac{\frac{1}{n} \sum_{j=1}^n f(\mathbf{B})_j f(\mathbf{B}_{\mathbf{A}}^{(i)})_j - \langle f(\mathbf{B}) \rangle \langle f(\mathbf{B}) \rangle}{\frac{1}{n} \sum_{j=0}^n f(\mathbf{B})_j f(\mathbf{B})_j - \langle f(\mathbf{B}) \rangle \langle f(\mathbf{B}) \rangle}. \quad (4)$$

Equation 3 is a corrected version; in the reference [6, Eq. 5.37] the estimate of  $\hat{E}^2$  should be the product of the mean of  $f(\mathbf{A})$  and the mean of  $f(\mathbf{B})$ .

The improved estimators [7] are calculated by:

$$S_i = \frac{\frac{1}{n} \sum_{j=1}^n f(\mathbf{A})_j (f(\mathbf{B}_{\mathbf{A}}^{(i)})_j - f(\mathbf{B})_j)}{\frac{1}{2n} \sum_{j=1}^{2n} f(\mathbf{C})_j f(\mathbf{C})_j - \langle f(\mathbf{C}) \rangle^2}, \quad (5)$$

$$T_i = \frac{\frac{1}{2n} \sum_{j=1}^{2n} (f(\mathbf{A})_j - f(\mathbf{B}_{\mathbf{A}}^{(i)})_j)^2}{\frac{1}{2n} \sum_{j=1}^{2n} f(\mathbf{C})_j f(\mathbf{C})_j - \langle f(\mathbf{C}) \rangle^2}. \quad (6)$$

The improved formula for the total sensitivity index is attributed to Jansen [2] by Saltelli et al. [7].

### Meta-models

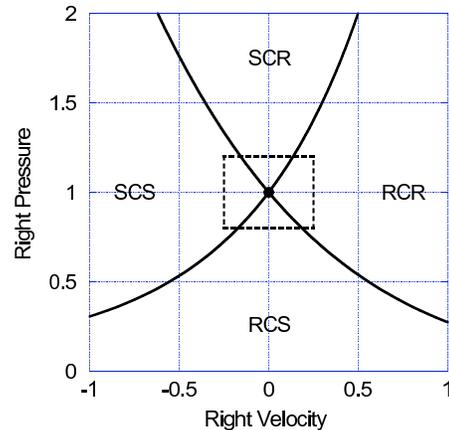
From a limited number of costly numerical simulations, a meta-model can be developed as a less expensive alternative. We consider three regression-based meta-models: State-Dependent Parameter Regression (SDP), the Adaptive Component Selection and Smoothing Operator (ACOSSO), and Design and Analysis of Computer Experiments (DACE). SDP models [3] are a class of non-parametric smoothing that is similar to smoothing splines and kernel regression approaches but is performed using a recursive Kalman filter approach with associated fixed interval smoothing. ACOSSO [8] is a multivariate smoothing-spline approach augmented by a weighted, scaled penalty function. The DACE approach is essentially the well-known Gaussian Process emulator.

Alternatively, stochastic expansion methods produce functional representations of stochastic variability, where model output is represented by analytic functions of stochastic inputs. We consider the Polynomial Chaos Expansion (PCE) [1], which represents the output as a sum of orthogonal polynomial basis functions, with the polynomials chosen according to the assumed input distribution. Once the coefficients of the polynomials are determined, one has an analytic formulation of the output. The stochastic expansion coefficients are used to directly calculate variance-based sensitivity indices. [9] This approach can be computationally efficient, insofar as the calculation of input sensitivities does not require additional function evaluations beyond those needed to construct the stochastic expansion.

### A Shock Physics Problem

The shock physics problem we consider is the one-dimensional shock tube problem for ideal gases. The governing equations are the inviscid Euler equations, which form the basis of many computational physics models. The Riemann problem is defined by two materials at initially

uniform states on both sides of an interface. When the interface is broken, the materials interact, generating waves. Three types of waves occur: rarefaction waves (smooth expansions), shock waves, and contact surfaces, the latter two of which involve discontinuous jumps across the wave. There are four possible wave configurations, as indicated in Fig. 1.



**Figure 1:** Map of the wave configurations of the shock tube problem, as a function of initial right pressure and velocity. The box identifies the region covered by these inputs in the sensitivity analysis problem. The sectors are identified by the solution structure, where “S” = shock, “C” = contact, and “R” = rarefaction.

### The Sensitivity Analysis Problem

For this study, the initial left state is held fixed at the values  $(\rho_L, p_L, u_L, \gamma_L) = (1.0, 1.0, 0.0, 1.4)$ , while the right density has a fixed value, 0.125, and the other inputs are given in Table I. A uniform distribution is assumed for all  $X_i$ . The computational domain,  $-0.5 \leq x \leq 1.5$  with the initial interface location is  $x = 0.5$ , is discretized into 200 elements. Simulations are run to a final time of  $t = 0.2$ . For a given set of input values, the ALEGRA code [4] is used to evaluate the numerical solution of the Riemann problem. The

**Table I: Input variables and their ranges.**

Input	Variable	Min.	Max.
$X_1$	$p_R$	0.8	1.2
$X_2$	$u_R$	-0.25	0.25
$X_3$	$\gamma_R$	1.2	1.6
$X_4$	CFL	0.8	1.2

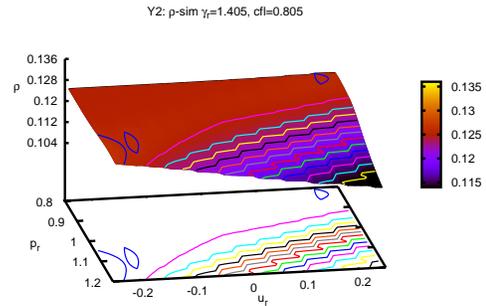
outputs  $Y_j, j = 1, \dots, 4$ , are extracted from the computed solution at fixed (Eulerian) spatial locations at the final time. Here we discuss only the second output, the density at  $x = 1.16$ .

Figure 2 shows the response surface for  $Y_2$  as a function of  $X_1$  and  $X_2$ , generated from the simulation model (ALEGRA). For low values of  $X_1$  and  $X_2$  no wave reaches this location, so  $Y_2$  retains its initial value. For high values, an expansion wave reduces the density by an amount that depends on the input values. Finally, with high values of  $X_1$  and low values of  $X_2$ , a shock reaches this location and the density is increased. Two FFS cases, generated using ALEGRA and labelled ‘‘AExact,’’ can be viewed as the exact solution to the sensitivity analysis problem using the simulation model.

A related sensitivity analysis problem is defined by using the exact solution of the Riemann problem (as apposed to approximate solutions from ALEGRA) to generate the response surface. We refer to this as the ‘‘exact model,’’ and two FFS cases, labelled ‘‘RExact,’’ are included in the results below.

### Preliminary Results

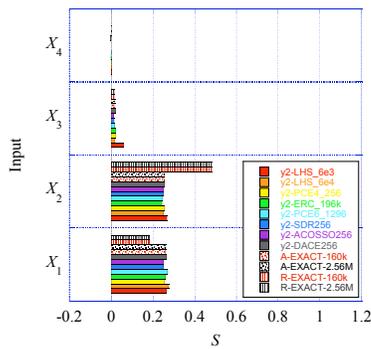
We conduct the sensitivity analyses with DAKOTA (<http://dakota.sandia.gov/>) from Sandia, and with SimLab (<http://simlab.jrc.ec.europa.eu/>) and other Matlab routines developed by JRC. One example of the results is Fig. 3, a plot of the main sensitivity indices  $S$  for the output  $Y_2$  (the final density at



**Figure 2: Response surface for  $Y_2$  from simulation with  $\gamma_R = 1.405$  and  $CFL = 0.805$ .**

$x = 1.16$ ), as estimated by several different methods and with different sample sizes. The corresponding total effects indices are shown in Fig. 4. There is obvious variability among the results for the different methods. In particular the ACOSSO and SDP underpredict the total effects for the three important inputs,  $X_1$ ,  $X_2$ , and  $X_3$ . Among the other methods there are slight but visible differences. For the important inputs the indices for for the main and total effects differ, with the total effects indices much greater than the main indices for almost every method, indicating that there are significant interaction effects among these inputs.

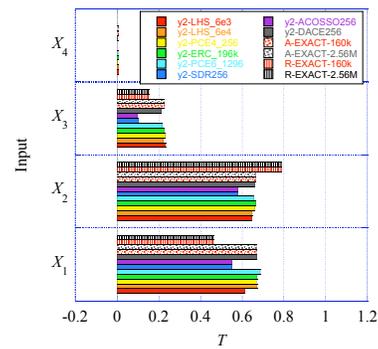
Additionally, this case exhibits a visible discrepancy between the full-factorial results for the exact model (‘‘RExact’’) and the simulation model (‘‘AExact’’) for both  $X_1$  and  $X_2$ . The exact model sensitivity indices for  $X_2$  are significantly greater than for  $X_1$  while these indices are essentially equal for the simulation model. This is a manifestation of the difference between the exact solution of the Riemann problem and the corresponding approximate numerical solution produced by the ALEGRA simulation code. Clearly, even for this weak shock problem, which is considered to be a very easy problem to simulate by the shock physics community, relatively small



**Figure 3: Main sensitivity index  $S$  for the output  $Y_2$  (final density at  $x = 1.16$ ).**

errors made in the simulations can influence the sensitivity analysis results.

In initial work on this article, the LHS results for 6000 and 60K samples were computed with the Saltelli et al. 2004 estimators (Eqs. (3) and (4)). Both  $S_i$  and  $T_i$  were quite inaccurate when calculated using 6000 or 60K samples, especially when compared to the other methods. We investigated this issue further, since it was a major concern: 60K samples should be sufficient to obtain accurate SA estimates for this 4-D problem, even with the interaction effects and nonlinearities. We compared two formulas for  $S_i$  and two formulas for  $T_i$ , as detailed in the first section. We analyzed this problem using five different seeds and 60K samples. Thus, for each seed, we generated a completely separate sensitivity analysis (involving  $10K \times (2 + 4) = 60K$  function evaluations for each seed). With each set of 60K samples, we computed  $S_i$  and  $T_i$  for both formulas. Further, for both the Saltelli et al. 2004 and the Saltelli et al. 2010 estimators, we computed the indices two ways: with the “true” function response and with the function response normalized by the mean (e.g., zero-mean function response).

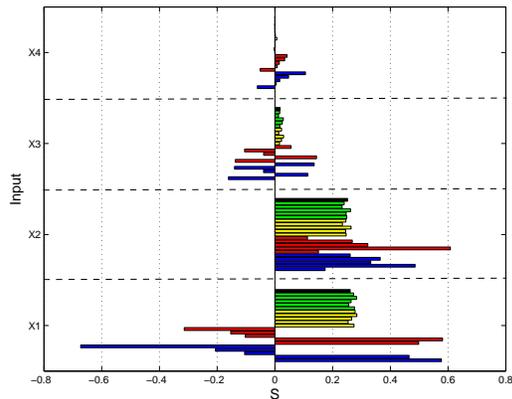


**Figure 4: Total sensitivity index  $T$  for the output  $Y_2$  (final density at  $x = 1.16$ ).**

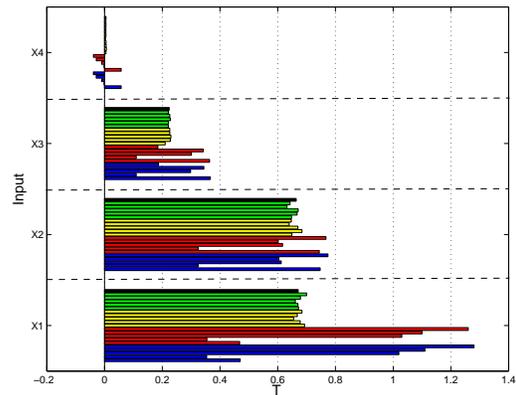
Figures 5 and 6 show the differences in the results for  $Y_2$ , a response that involves significant interaction between the inputs. The exact values of  $S_i$  are 0.26, 0.25, 0.02,  $2.0 \times 10^{-4}$  for variables  $X_1$ – $X_4$ , respectively. The exact values of  $T_i$  are 0.67, 0.66, 0.2, and 0.005 for variables  $X_1$ – $X_4$ , respectively. Figure 5 shows that the formulas with a normalized response (yellow and green bars) clearly perform better than the un-normalized formulas shown by the red and blue bars. This is true for both  $S_i$  and  $T_i$  (shown in Fig. 6) but especially for  $S_i$ . Without normalizing the responses, the main effects indices are often negative, which indicates erroneous results. In the normalized cases, there are very slight differences between the 2004 and 2010 implementations (green and yellow), but in quantitative comparisons the 2010 formulas are more accurate and show more consistency (lack of variability across seeds.)

## Conclusions

We have compared several different sensitivity analysis approaches for a canonical shock physics problem. We examine variance-based Sobol’ sensitivity indices produced by these approaches to learn how well they perform as a function of the number of samples and how accurate they are for



**Figure 5: Main sensitivity index  $S_i$  for  $Y_2$  (final density at  $x = 1.16$ ) from two estimators, with and without normalization, and five independent LHS designs. The black bar for each input (above the green bars) is the exact result from “AExact 2.56M”. Blue bars are from Saltelli et al. 2004, Eq. (3), *not* normalized. Red bars are from Saltelli et al. 2010, Eq. (5), *not* normalized. Yellow bars are from Saltelli et al. 2004, Eq. (3), normalized. Green bars are from Saltelli et al. 2010, Eq. (5), normalized.**



**Figure 6: Total sensitivity index  $T_i$  for  $Y_2$  (final density at  $x = 1.16$ ) from two estimators, with and without normalization, and five independent LHS designs. The black bar for each input (above the green bars) is the exact result from “AExact 2.56M”. Blue bars are from Saltelli et al. 2004, Eq. (4), *not* normalized. Red bars are from Saltelli et al. 2010, Eq. (6), *not* normalized. Yellow bars are from Saltelli et al. 2004, Eq. (4), normalized. Green bars are from Saltelli et al. 2010, Eq. (6), normalized.**

discontinuous response surfaces. Our simulation model provides approximate numerical solutions to this problem, and can be executed quickly enough to generate as many samples as needed. This allows us to use a full factorial sampling of the input hypercube to provide exact sensitivity indices, to which we compare the estimates from the sampling and meta-modeling approaches.

1. The number of samples used for this initial work was sufficient to obtain accurate sensitivity indices from all the methods. Overall the different sampling approaches and meta-models gave similar results, with the DACE and PCE meta-models slightly better than SDP and ACOSSO when

interactions among inputs were significant.

2. For LHS sampling, a detail about how the estimators are applied makes a big difference in the results for outputs with interacting inputs. In particular, it is critical to subtract the mean value of the output before applying the sensitivity index estimators (Eqs. (3), (4), (5), and (6).) Without this step, there was very little consistency in the index values across independent LHS designs, and this inconsistency was much greater than the differences between the Saltelli et al. 2004 and Saltelli et al. 2010 formulas. The 2010 formulas are more accurate than the 2004 formulas.

3. Our shock physics problem has a known, exact solution. When this exact model replaces the simulation model (which provides *approximate* numerical solutions), for some outputs the sensitivity indices change significantly. While this does not affect our examination of the different techniques, it does emphasize the risks of drawing inferences about reality based on models of reality.

A more detailed description of this work has been submitted to Reliability Engineering & System Safety for publication. We intend to build upon these results in several ways. We intend to examine more complicated physics problems that involve discontinuous behavior. Additionally, we plan to extend the methodologies discussed in this work to discontinuous inputs; such inputs are widespread in multiphysics simulation codes, which often allow, for example, different numerical methods, different models for the physics, and different databases for material response. Although there were not striking differences among the different methods used to estimate sensitivity indices for the idealized problem examined of this study, we speculate that greater differences between approaches will be seen as discrete inputs are incorporated.

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