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Survey of sampling-based methods for uncertainty and sensitivity analysis

J.C. Helton[a,*], J.D. Johnson[b], C.J. Sallaberry[c], C.B. Storlie[d]

[a]Department of Mathematics and Statistics, Arizona State University, Tempe, AZ 85287-1804, USA
[b]ProStat, Mesa, AZ 85204-5326, USA
[c]Sandia National Laboratories, Albuquerque, NM 87185-0776, USA
[d]Department of Statistics, Colorado State University, Fort Collins, CO 80523-1877, USA

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Abstract

Sampling-based methods for uncertainty and sensitivity analysis are reviewed. The following topics are considered: (i) definition of probability distributions to characterize epistemic uncertainty in analysis inputs, (ii) generation of samples from uncertain analysis inputs, (iii) propagation of sampled inputs through an analysis, (iv) presentation of uncertainty analysis results, and (v) determination of sensitivity analysis results. Special attention is given to the determination of sensitivity analysis results, with brief descriptions and illustrations given for the following procedures/techniques: examination of scatterplots, correlation analysis, regression analysis, partial correlation analysis, rank transformations, statistical tests for patterns based on gridding, entropy tests for patterns based on gridding, nonparametric regression analysis, squared rank differences/rank correlation coefficient test, two-dimensional Kolmogorov–Smirnov test, tests for patterns based on distance measures, top down coefficient of concordance, and variance decomposition.

Keywords: Aleatory uncertainty; Epistemic uncertainty; Latin hypercube sampling; Monte Carlo; Sensitivity analysis; Uncertainty analysis

1. Introduction

Uncertainty analysis and sensitivity analysis are essential parts of analyses for complex systems [1–14]. Specifically, uncertainty analysis refers to the determination of the uncertainty in analysis results that derives from uncertainty in analysis inputs, and sensitivity analysis refers to the determination of the contributions of individual uncertain analysis inputs to the uncertainty in analysis results. The uncertainty under consideration here is often referred to as epistemic uncertainty; alternative designations for this form of uncertainty include state of knowledge, subjective, reducible, and type B [15–24]. Epistemic uncertainty derives from a lack of knowledge about the appropriate value to use for a quantity that is assumed to have a fixed value in the context of a particular analysis. In the conceptual and computational organization of an analysis, epistemic uncertainty is generally considered to be distinct from aleatory uncertainty, which arises from an inherent randomness in the behavior of the system under study [15–24]. Alternative designations for aleatory uncertainty include variability, stochastic, irreducible, and type A.

A number of approaches to uncertainty and sensitivity analysis have been developed, including differential analysis [25–33], response surface methodology [34–43], Monte Carlo analysis [44–55], and variance decomposition procedures [56–60]. Overviews of these approaches are available in several reviews [61–68].

The focus of this presentation is on Monte Carlo (i.e., sampling-based) approaches to uncertainty and sensitivity analysis. Sampling-based approaches to uncertainty and sensitivity analysis are both effective and widely used [69–83]. Analyses of this type involve the generation and exploration of a mapping from uncertain analysis inputs to uncertain analysis results. The underlying idea is that analysis results $\mathbf{y}(\mathbf{x}) = [y_1(\mathbf{x}), y_2(\mathbf{x}), \ldots, y_{nY}(\mathbf{x})]$ are functions of uncertain analysis inputs $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$. In

*Corresponding author. Sandia National Laboratories, Department 6849, MS 0779, Albuquerque, NM, 87185-0779, USA.
Tel.: +1 505 284 4808; fax: +1 505 844 2348.
E-mail address: jchelto@sandia.gov (J.C. Helton).

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turn, uncertainty in $\mathbf{x}$ results in a corresponding uncertainty in $\mathbf{y}(\mathbf{x})$. This leads to two questions: (i) what is the uncertainty in $\mathbf{y}(\mathbf{x})$ given the uncertainty in $\mathbf{x}$? and (ii) how important are the individual elements of $\mathbf{x}$ with respect to the uncertainty in $\mathbf{y}(\mathbf{x})$? The goal of uncertainty analysis is to answer the first question, and the goal of sensitivity analysis is to answer the second question. In practice, the implementation of an uncertainty analysis and the implementation of a sensitivity analysis are very closely connected on both a conceptual and a computational level.

The following sections summarize and illustrate the five basic components that underlie the implementation of a sampling-based uncertainty and sensitivity analysis: (i) definition of distributions $D_1, D_2, \ldots, D_{nX}$ that characterize the epistemic uncertainty in the elements $x_1, x_2, \ldots, x_{nX}$ of $\mathbf{x}$ (Section 2), (ii) generation of a sample $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_{nS}$ from the $\mathbf{x}$'s in consistency with the distributions $D_1, D_2, \ldots, D_{nX}$ (Section 3), (iii) propagation of the sample through the analysis to produce a mapping $[\mathbf{x}_i, \mathbf{y}(\mathbf{x}_i)]$, $i = 1, 2, \ldots, nS$, from analysis inputs to analysis results (Section 4), (iv) presentation of uncertainty analysis results (i.e., approximations to the distributions of the elements of $\mathbf{y}$ constructed from the corresponding elements of $\mathbf{y}(\mathbf{x}_i)$, $i = 1, 2, \ldots, nS$) (Section 5), and (v) determination of sensitivity analysis results (i.e., exploration of the mapping $[\mathbf{x}_i, \mathbf{y}(\mathbf{x}_i)]$, $i = 1, 2, \ldots, nS$) (Section 6). The presentation then ends with a concluding summary (Section 7).

Only probabilistic characterizations of uncertainty are considered in this presentation. Alternative uncertainty representations (e.g., evidence theory, possibility theory, fuzzy set theory, interval analysis) are active areas of research [84–92] but are outside the intended scope of this presentation.

2. Characterization of uncertainty

Definition of the distributions $D_1, D_2, \ldots, D_{nX}$ that characterize the epistemic uncertainty in the elements $x_1, x_2, \ldots, x_{nX}$ of $\mathbf{x}$ is the most important part of a sampling-based uncertainty and sensitivity analysis as these distributions determine both the uncertainty in $\mathbf{y}$ and the sensitivity of the elements of $\mathbf{y}$ to the elements of $\mathbf{x}$. The distributions $D_1, D_2, \ldots, D_{nX}$ are typically defined through an expert review process [93–100], and their development can constitute a major analysis cost. A possible analysis strategy is to perform an initial exploratory analysis with rather crude definitions for $D_1, D_2, \ldots, D_{nX}$ and use sensitivity analysis to identify the most important analysis inputs; then, resources can be concentrated on characterizing the uncertainty in these inputs and a second presentation or decision-aiding analysis can be carried out with these improved uncertainty characterizations.

The scope of an expert review process can vary widely depending on the purpose of the analysis, the size of the analysis, and the resources available to carry out the analysis. At one extreme is a relatively small study in which a single analyst both develops the uncertainty characterizations (e.g., on the basis of personal knowledge or a cursory literature review) and carries out the analysis. At the other extreme, is a large analysis on which important societal decisions will be based and for which uncertainty characterizations are carried out for a large number of variables by teams of outside experts who support the analysts actually performing the analysis.

Given the breadth of analysis possibilities, it is beyond the scope of this presentation to provide an exhaustive review of how the distributions $D_1, D_2, \ldots, D_{nX}$ might be developed. However, as general guidance, it is best to avoid trying to obtain these distributions by specifying the defining parameters (e.g., mean and standard deviation) for a particular distribution type. Rather, distributions can be defined by specifying selected quantiles (e.g., 0.0, 0.1, 0.25,…,0.9, 1.0) of the corresponding cumulative distribution functions (CDFs), which should keep the individual supplying the information in closer contact with the original sources of information or insight than is the case when a particular named distribution is specified (Fig. 1a). Distributions from multiple experts can be aggregated by averaging (Fig. 1b) [101].

This presentation draws most of its examples from an uncertainty and sensitivity analysis carried out for a two phase flow model (implemented in the BRAGFLO program) [102–104] in support of the 1996 Compliance Certification Application for the Waste Isolation Pilot Plant [105–107]. The uncertain variables considered in the example results (i.e., $x_1, x_2, \ldots, x_{nX}$ with $nX = 31$) and their associated distributions (i.e., $D_1, D_2, \ldots, D_{31}$) are summarized in Table 1. Additional information on the use of these variables in the two phase flow model and on the development of the associated uncertainty distributions is available in the original analysis documentation [102,108].

Additional information: Section 6.2, Refs. [46, 93–100,109–119]. As an example, Ref. [100] describes the approach used in the extensive expert review process that supported the US Nuclear Regulatory Commission's (NRC's) reassessment of the risk from commercial nuclear power plants (i.e., NUREG-1150; see Refs. [82,120–124]).

3. Generation of sample

Several sampling strategies are available, including random sampling, importance sampling, and Latin hypercube sampling [44,55] Latin hypercube sampling is very popular for use with computationally demanding models because its efficient stratification properties allow for the extraction of a large amount of uncertainty and sensitivity information with a relatively small sample size.

Latin hypercube sampling operates in the following manner to generate a sample of size nS from the distributions $D_1, D_2, \ldots, D_{nX}$ associated with the elements of $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$. The range of each x_j is exhaustively divided into nS disjoint intervals of equal probability and one value x_{ij} is randomly selected from each interval. The nS values for x_1 are randomly paired without replacement