Sampling-Based Methods for Uncertainty and Sensitivity Analysis

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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.

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

1. INTRODUCTION

Sampling-based (i.e., Monte Carlo) approaches to uncertainty and sensitivity analysis are both effective and widely used [1-4]. 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 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 questions. 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 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 uncertainty in the components $x_1, x_2, \ldots, x_{nX}$ of $\mathbf{x}$ (Sect. 2), (ii) Generation of a sample $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_{nS}$ fro the $\mathbf{x}$'s in consistency with the distributions $D_1, D_2, \ldots, D_{nX}$ (Sect. 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 (Sect. 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 $\mathbf{y}(\mathbf{x}_i)$, $i = 1, 2, \ldots, nS$) (Sect. 5), and (v) Determination of sensitivity analysis results (i.e., exploration of the mapping $[\mathbf{x}_i, \mathbf{y}(\mathbf{x}_i)]$, $i = 1, 2, \ldots, nS$) (Sect. 6). Space limitations in this presentation preclude the presentation of detailed examples of the indicated analysis components; however, examples can be found in the published descriptions of an uncertainty and sensitivity analysis carried out for the Waste

Sensitivity Analysis of Model Output
Kenneth M. Hanson and François M. Hemez, eds.
Los Alamos National Laboratory, 2005; http://library.lanl.gov/

Isolation Pilot Plant (e.g., [5-7]). The presentation then ends with a concluding summary (Sect. 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 an active area of research [8, 9] but are outside the intended scope of this presentation.

2. CHARACTERIZATION UNCERTAINTY

Definition of the distributions $D_1, D_2, \ldots, D_{nX}$ that characterize the uncertainty in the components $x_1, x_2, \ldots, x_{nX}$ of $\mathbf{x}$ is the most important part of a sampling-based uncertainty and sensitivity analysis as these distributions determine both the uncertainty in y and the sensitivity 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 [10-13], 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). 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 define these distributions by specifying the defining parameters (e.g., mean and standard deviation) for a particular distribution. Rather, distributions can be defined by specifying selected quantiles (e.g., 0.0, 0.1, 0.25, …, 0.9, 1.0), 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. Distributions from multiple experts can be aggregated by averaging.

3. GENERATION OF SAMPLE

Several sampling strategies are available, including random sampling, importance sampling, and Latin hypercube sampling [14, 15]. 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 with the nS value for x_2 to produce nS pairs. These pairs are then randomly combined without replacement with the nS values for x_3 to produce nS triples. This process is continued until a set of nS nX-triples $\mathbf{x}_i = [x_{i1}, x_{i2}, \ldots, x_{i,nX}]$, $i = 1, 2, \ldots, nS$, is obtained, with this set constituting the Latin hypercube sample. In addition, effective correlation control procedures are available for use with Latin hypercube sampling [16, 17]. The popularity of Latin hypercube sampling recently led to the original article being designated a *Technometrics* classic in experimental design [18].

Latin hypercube sampling is a good choice for a sampling procedure when computationally demanding models are being studied. When the model is not computationally demanding, many model evaluations can be performed and random sampling works as well as Latin hypercube sampling.

4. PROPAGATION OF SAMPLE THROUGH THE ANALYSIS

Propagation of the sample through the analysis to produce the mapping $[\mathbf{x}_i, \mathbf{y}(\mathbf{x}_i))]$, $i = 1, 2, \ldots, nS$, from analysis inputs to analysis results is often the most computationally demanding part of a sampling-based uncertainty and sensitivity analysis. The details of this propagation are analysis specific and can range from very simple for analyses that involve a single model to very complicated for large analyses that involve complex systems of linked models [7, 19].

When a single model is under consideration, this part of the analysis can involve little more than putting a DO loop around the model that (i) supplies the sampled input to the model, (ii) runs the model, and (iii) stores model results for later analysis. When more complex analyses with multiple models are involved, considerable sophistication may be required in this part of the analysis. Implementation of such analyses can involve (i) development of simplified models to approximate more complex models, (ii) clustering of results at model interfaces, (ii) reuse of model results through interpolation or linearity properties, and (iv) complex procedures for the storage and retrieval of analysis results.

5. PRESENTATION OF UNCERTAINTY ANALYSIS RESULTS

Presentation of uncertainty analysis results is generally straight forward and involves little more than displaying the results associated with the already calculated mapping $[\mathbf{x}_i, \mathbf{y}(\mathbf{x}_i)]$, $i = 1, 2, \ldots, nS$. Presentation possibilities include means and standard deviations, density functions, cumulative distribution function (CDFs), complementary cumulative distribution functions (CCDFs), and box plots [2, 15]. Presentation formats such as CDFs, CCDFs and box plots are usually preferable to means and standard deviations because of the large amount of uncertainty information that is lost in the calculation of means and standard deviations.

6. DETERMINATION OF SENSITIVITY ANALYSIS RESULTS

Determination of sensitivity analysis results is usually more demanding that the presentation of uncertainty analysis results due to the need to actually explore the mapping $[\mathbf{x}_i, \mathbf{y}(\mathbf{x}_i)]$, $i = 1, 2, \ldots, nS$, to assess the effects of individual components of $\mathbf{x}$ on the components of $\mathbf{y}$. A number of approaches to sensitivity analysis that can be used in conjunction with a sampling-based uncertainty analysis are listed and briefly summarized below. In this summary, (i) x_j is an element of $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$, (ii) y_k is an element of $\mathbf{y}(\mathbf{x}) = [y_1(\mathbf{x}), y_2(\mathbf{x}), \ldots, y_{nY}(\mathbf{x})]$, (iii) $\mathbf{x}_i = [x_{i1}, x_{i2}, \ldots, x_{i,nX}]$, $i = 1, 2, \ldots, nS$, is a random or Latin hypercube sample from the possible values for $\mathbf{x}$ generated in consistency with the joint distribution assigned to the x_j, (iv) $\mathbf{y}_i = \mathbf{y}(\mathbf{x}_i)$ for $i = 1, 2, \ldots, nS$, and (v) x_{ij} and y_{ik} are arbitrary elements of $\mathbf{x}_i$ and $\mathbf{y}_i$, respectively.

Scatterplots. Plots of points $[x_{ij}, y_{ik}]$ for $i = 1, 2, \ldots, nS$ can reveal nonlinear or other unexpected relationships. Natural starting point in complex analysis that can help development of sensitivity analysis strategy using one or more additional techniques. Additional information: Sect. 6.6.1, [20].

Cobweb Plots. Plots of points $[\mathbf{x}_i, y_{ik}] = [x_{i1}, x_{i2}, \ldots, x_{i,nX}, y_{ik}]$ for $i = 1, 2, \ldots, nS$. Provides two-dimensional representation for a $nX + 1$ dimensional quantity. Generalization of a scatterplot. Provides more information in a single plot frame than a scatterplot but is harder to read. Additional information: Sect. 11.7, [21]

Correlation. Provides measure of the strength of the linear relationship between x_j and y_k. Equal to standardized regression coefficient in linear regression relating y_k to x_j; also equal in absolute value to the square root of the R^2 value associated with the indicated regression. Often referred to as Pearson correlation coefficient. Additional information: Sect. 6.6.4, [20].

Regression Analysis. Provides algebraic representation of relationships between y_k and one or more x_j's. Usually performed in stepwise fashion with initial inclusion of most important x_j, then two most important x_j's, and so on until no more x_j's that significantly affect y_k can be identified. Variable importance indicated by order of selection in stepwise process, changes in R^2 values as additional variables are added to the regression model, and standardized regression coefficients for the x_j's in the final regression model. Additional information: Sects. 6.6.2, 6.6.3, 6.6.5, [20].

Partial Correlation. Provides measure of the strength of the linear relationship between y_k and x_j after the linear effects of all other elements of $\mathbf{x}$ have been removed. Additional information: Sect. 6.6.4, [20].

Rank Transformations. Replaces values for y_k and x_j with their corresponding ranks. Smallest valued assigned a rank of 1; next largest value assigned a rank of 2; tied values are assigned their average rank; and so on up to the largest value, which is assigned a rank of nS. Converts a nonlinear but monotonic relationship between y_k and x_j to a linear relationship. Produces rank (i.e., Spearman) correlations, rank regressions, standardized rank regression coefficients and partial rank correlation coefficients. Additional information: Sect. 6.6.6, [20]; [22].

Nonparametric Regression. Seeks more general models than those obtained by least squares regression. Attempts to find models that are local in the approximation to the relationship between y_k and multiple x_j's. Better at capturing complex nonlinear relationships than traditional regression or rank regression. Can be applied in stepwise manner. Sequential changes in R^2 values with addition of successive variables to the model provides indication of variable importance. Very promising. Additional information: [23-25].

Tests for Patterns Based on Gridding. Grids can be placed on the scatterplot for y_k and x_j and then various statistical tests can be performed to determine if the distribution of points across the grid cells appears to be nonrandom. Appearance of a nonrandom pattern indicates that x_j has an effect on y_k. Possibilities include (i) tests for common means, common medians, and common distributions for values of y_k based on partitioning the range of x_j and (ii) tests for no influence based on partitioning the ranges of x_j and y_k. Additional information: Sects. 6.6.8, 6.6.9, [20]; [26].

Tests for Patterns Based on Distance Measures. Considers relationships within the scatterplot for y_k and x_j such as the distribution of distances between nearest neighbors. Provides way to identify nonrandom relationships between y_k and x_j. Avoids problem of defining appropriate gridding associated grid-based methods. Additional information: [27-30].

Trees. Searches for relationships between y_k and multiple x_j's by successively subdividing the sample elements $\mathbf{x}_i$ on the basis of observed effects of individual x_j's on y_k. Additional information: [31].

Two-Dimensional Kolmogorov-Smirnov Test. Provides way to test for nonrandom patterns in the scatterplot for y_k and x_j that does not require the imposition of a grid. Additional information: [32-34].

Squared Differences of Ranks. Seeks to identify presence of nonlinear relationship between y_k and x_j. Based on squared differences of consecutive ranks of y_k when the values of y_k have been ordered by the corresponding values of x_j. Additional information: [35].

Top-Down Concordance with Replicated Samples. Uses top-down coefficient of concordance and replicated (i.e., independently generated) samples. Sensitivity analysis with some appropriate technique performed for each sample. Top-down coefficient used to identify important variables by seeking variables with similar rankings across all replicates. Additional information: [36].

Variance Decomposition. The variance decomposition proposed by Sobol' and others is formally defined by high-dimensional integrals involving the x_j and $y_k(\mathbf{x})$. Provides decomposition of variance $V(y_k)$ of y_k in terms of the contributions V_j of individual x_j's to $V(y_k)$ and also the contributions of various interactions between the x_j to $V(y_k)$. In practice, indicated decomposition is obtained with sampling based methods. Two samples from $\mathbf{x}$ of size nS are required to estimate all V_j; $nX + 2$ samples of size nS are required to estimate all V_j and also the contributions of each of the x_j's and its interactions with other elements of $\mathbf{x}$ to $V(y_k)$. Conceptually very appealing but can be computationally demanding as more samples and probably larger samples required than with other sampling-based approaches to sensitivity analysis. Additional information: [37, 38]

7. SUMMARY

Sampling-based uncertainty and sensitivity analysis is widely used, and as a result, is a fairly mature area of study. However, there still remain a number of important challenges and areas for additional study. For example, there is a need for sensitivity analysis procedures that are more effective at revealing nonlinear relations than those currently in use. Among the approaches to sensitivity analysis listed in Sect. 6, nonparametric regression [23-25], the two-dimensional Kolmogorov-Smirnov test [32-34], tests for nonmonotone relations [35], tests for nonrandom patterns [26-30], and complete variance decomposition [37, 38] have not been as widely used as some of the other approaches and merit additional investigation and use. As another example, sampling-based procedures for uncertainty and sensitivity analysis usually use probability as the model, or representation, for uncertainty. However, when limited information is available with which to characterize uncertainty, probabilistic characterizations can give the appearance of more knowledge than is really present. Alternative representations for uncertainty such as evidence theory and possibility theory merit consideration for their potential to represent uncertainty in situations where little information is available [8, 9]. Finally, a significant challenge is the education of potential users of uncertainty and sensitivity analysis about (i) the importance of such analyses and their role in both large and small analyses, (ii) the need for appropriate separation of aleatory and epistemic uncertainty in the conceptual and computational implementation of analyses of complex systems [39-43], (ii) the need for a clear conceptual view of what an analysis is intended to represent and a computational design that is consistent with that view [44], (iv) the role that uncertainty and sensitivity analysis plays in model and analysis verification, and (v) the importance of avoiding deliberately conservative assumptions if meaningful uncertainty and sensitivity analysis results are to be obtained.

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