Key Criteria and Selection of Sensitivity Analysis Methods Applied to Natural Resource Models

[1]Ascough II, J.C., T.R. Green, L. Ma, and L.R. Ahjua

[1]USDA-ARS, Great Plains Systems Research Unit, Fort Collins, CO 80526
E-Mail: jim.ascough@ars.usda.gov

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EXTENDED ABSTRACT

Integrated natural resource models (e.g., APSIM) are typically large and complex, thus, it can be difficult to prioritize parameters that are most promising with respect to system management goals. It is important to evaluate how a model responds to changes in its inputs as part of the process of model development, verification, and evaluation. There are several techniques for sensitivity analysis used by practitioners and analysts in numerous fields. For example, sensitivity analysis methods are commonly built-in features of a particular software tool, e.g., Crystal Ball or @Risk. However, there are other sensitivity analysis methods, including those used outside of the natural resources field, applicable to integrated system models. In this paper, we concentrate on qualitatively evaluating four sensitivity analysis methods: 1) Fourier Amplitude Sensitivity Test (FAST), 2) Response Surface Method (RSM), 3) Mutual Information Index (MII), and 4) the methods of Sobol'. For sensitivity analysis of natural resource models, the FAST and Sobol' methods are particularly attractive. These methods are capable of computing the so-called "Total Sensitivity Indices" (TSI), which measure parameter main effects and all of the interactions (of any order) involving that parameter.

Additional recommendations resulting from our evaluation include:

- Sensitivity analysis should be used prior to model development, during model development, and when the model is applied to a specific problem.
- Sensitivity analysis provides useful risk insights, but alternative approaches are also needed to understand "which" parameters show up as important and "why" they show up as important.
- Sensitivity analysis can be a valuable tool in building confidence in the model and in the embedded computer codes.
- In spite of current advances, the state-of-the-science has not matured to the point of quantitatively deriving significance from sensitivity analyses as input to final decision-making.
- The use of global sensitivity methods is emphasized herein. Many methods currently in use have some sort of global aspect (though not explicitly recognized), in particular, variance-based sensitivity measures (e.g., FAST and Sobol') are concise and easy to understand and communicate.

There is a concern that uncertainty and sensitivity analysis methods could be incorrectly used to make a case for or against a project. Therefore, there is a need to develop guidance documents (with expert involvement or endorsement) that will provide sensitivity analysis practitioners with knowledge of what is available, and the context of where the methods can be used (i.e., when to use them, and how to use them). Recent developments illustrate the tremendous need for implementing quantitative sensitivity analyses. Furthermore, a gap remains in public education of the utility and implementation of sensitivity analysis methods in the decision-making process.

Issues addressed in this paper pertaining to the application of sensitivity analysis in natural resource modeling include: 1) criteria for sensitivity analysis methods applied to natural resource models, 2) identification of several promising sensitivity analysis methods for application to natural resource models, and 3) needs for implementation and demonstration of sensitivity analysis methods. As stated above, it is our goal that this paper will eventually lead to creation of a guidance document for assisting practitioners with regard to the selection of sensitivity analysis methods, and their application, interpretation, and reporting. The overall guidelines should not be too restrictive, but instead provide useful boundaries and principles for selecting, using, and interpreting results from sensitivity analysis methods.

1. INTRODUCTION

Mathematical models are commonly developed to approximate engineering, biological, chemical, physical, environmental, and socioeconomic phenomena of varying complexity. Model development usually consists of several logical steps, one of which should be the determination of model input parameters which most influence model output. Sensitivity analysis is the study of how the uncertainty in the output of a model can be allocated to different sources of uncertainty in the model input. Therefore, sensitivity analysis is considered by some as a prerequisite for model building in any setting, be it diagnostic or predictive, and in any research area where mathematical models are used. Furthermore, a sensitivity analysis of model input parameters can serve as a guide to any further application of the model. Quantitative sensitivity analysis is being invoked increasingly for corroboration, quality assurance, and the defensibility of model-based analyses.

Sensitivity analysis can be used as an aid in identifying the important uncertainties for the purpose of prioritizing additional data collection or research (Frey et al., 2004). In addition, sensitivity analysis can play an important role in model verification and validation throughout the course of model development and refinement (e.g., Kleijnen and Sargent, 2000; Fraedrich and Goldberg, 2000). Sensitivity analysis also can be used to provide insight into the robustness of model results when making decisions (Saltelli et al., 2000). In general, modelers conduct sensitivity analysis for a number of reasons including the desire to determine:

1. Which input parameters contribute the most to output variability, thereby requiring additional research to increase knowledge of parameter behavior in order to reduce output uncertainty;
2. If parameter interactions are present, which (group of) parameters interact with each other;
3. Which parameters are insignificant and can be held constant or eliminated from the final model; and
4. The optimal regions within the parameter space for use in subsequent calibration studies.

Sensitivity analysis methods have been applied in various research fields, including complex engineering systems, economics, physics, social sciences, medical decision making, and others (e.g., Helton, 1993; Merz et al., 1992).

Issues to be addressed in this paper pertaining to the application of sensitivity analysis in natural resource modeling include: 1) criteria for sensitivity analysis methods applied to natural resource models, 2) identification of promising sensitivity analysis methods for application to natural resource models, and 3) research needs for implementation and demonstration of sensitivity analysis methods. Specific questions that a practitioner should ask with regard to the above three issues include (Frey et al., 2004):

- When should sensitivity analysis be performed?
- How should a model be prepared to facilitate sensitivity analysis?
- What are some typical sensitivity analysis methods?
- How should particular sensitivity analysis methods be selected, and how should the methods be applied?
- How should the results of sensitivity analysis be presented and interpreted?

It is beyond the scope of this manuscript to answer all of these questions. However, we endeavor to investigate some of them in the hope that this paper will eventually lead to creation of a guidance document for assisting natural resource modeling practitioners with regard to the selection of sensitivity analysis methods, their application, interpretation, and reporting.

2. SENSITIVITY ANALYSIS MODELING ISSUES

Frey et al. (2004) define sensitivity analysis as the assessment of the impact of changes in input values on model outputs. Similarly, Saltelli et al. (2000) define sensitivity analysis as the study of how the variation in the output of a model can be apportioned, qualitatively or quantitatively, among model inputs. The answers sought from application of sensitivity analysis should always be clearly listed. The usefulness of sensitivity analysis can then be assessed based on whether the available methods of sensitivity analysis can address the questions under consideration in a manner that is appropriate to the characteristics of the model. Key motivations for performing a sensitivity analysis include identification of key sources of variability and uncertainty in order to facilitate model development, verification, and validation; prioritization of key sources of variability and uncertainty in order to prioritize additional data collection and research; and general model refinement (Frey et al., 2004).

2.1 Model Suitability Study

Prior to application of any sensitivity analysis methods, the model under study should be evaluated as to suitability for the analysis. In particular, it is important that the model is programmed in a manner such that the inputs and outputs are clearly identifiable and accessible. Furthermore, inherent characteristics of the model (e.g., modularity, stochastic vs. deterministic) may constrain the use of particular sensitivity analysis methods. Sensitivity analysis should be included in the list of primary modeling objectives at the time of model development. The implementation of specific model development strategies will facilitate sensitivity analysis. For an existing model, the practitioner is typically interested in applying sensitivity analysis with minimum modification to the model. However, in some situations, if the model has not been designed to facilitate sensitivity analysis, substantial modifications may be required (Frey and Patil, 2002). Generally, a thorough understanding of the model and its limitations is essential to select well-suited sensitivity analysis methods and to determine the scope of sensitivity analysis application. The scope of sensitivity analysis may include the entire model or could be focused on specific modules or parts of a model.

Model characteristics have a critical influence on the choice of sensitivity analysis methods and the scope of sensitivity analysis. In many (if not most) cases, modelers might not have anticipated the application of sensitivity analysis, and hence, the model may not have been developed in a manner that facilitates sensitivity analysis. To identify whether the modeling methodology used is compatible with application of sensitivity analysis, the model has to be thoroughly reviewed and characterized. Key features that need to be studied in the process of understanding a model (in the context of sensitivity analysis) include:

- *Identification of model structure*: This helps determine the scope of sensitivity analysis.

- *Identification of inputs*: The inputs of interest must be identified to perform a sensitivity analysis - model inputs may represent variability, uncertainty, or both.

- *Selection of model output responses for sensitivity analysis*: This is frequently highly dependent on the assessment objectives.

- *Simulation design*: Performing a simulation is a prior step to application of any sensitivity analysis method; results obtained from sensitivity analysis are directly related to the characteristics and the scope of the simulation.

- *Model modification*: In some situations a model must be modified to apply sensitivity analysis - these modifications often demand changing data storage procedures (e.g., model inputs, outputs, and internal inputs).

2.2. Determining Sources of Variability and Uncertainty

In order to prioritize data collection activities, it is useful to prioritize the key sources of uncertainty and variability through a sensitivity analysis. In many cases, the overall variability in a model output response is influenced by only a small subset of model inputs that are subject to variability. Similarly, the uncertainty in a selected model output response may be influenced by only a subset of the model inputs that are subject to uncertainty. Sensitivity analysis can be applied to a model to provide insight regarding which model inputs contribute the most to uncertainty, variability, or both, for a particular model output. This insight can then be used to allocate scarce resources preferentially to data collection or research for those inputs that matter the most for model application. In the case of uncertainty, the collection of additional data collection or research may be the only viable method for reducing the uncertainty. In the case of variability, the collection of additional data can be used to develop more accurate estimates of variability through acquisition of data with better quality (e.g., improved representation), and can reduce uncertainty about potential bias in the most important variable inputs. Obviously, it may not be feasible to collect additional data in some cases. In these situations, sensitivity analysis can provide insight regarding the robustness of the model output with regard to variation in a model input; whether due to uncertainty, variability, or both.

2.3 Model Development, Evaluation, and Refinement

During the process of developing or refining a model, sensitivity analysis can be used as a confidence building measure with regard to model credibility. Quantitative sensitivity analysis is increasingly invoked for verification and validation of model-based analysis (Saltelli, 2002a). Sensitivity analysis can be helpful in verification and validation of a model. In particular, the objective of sensitivity analysis applied to model verification is to assess whether the model output responds appropriately to a change in model inputs. Sensitivity analysis also can assist in the validation process. For example, if a model output responds by only 1% to a 25% change in a particular input, then it may not be important to have an accurate estimate for that particular input. In contrast, if a model output varies by 25% if a particular input changes by only 1%, then it could be critically important to specify an accurate value for that input as part of a validation exercise. Sensitivity analysis is helpful not only as a critique to model development as part of verification and validation, but also to guide model development. The identification of inputs that are of insignificant importance to the variation in the output could be used to guide the elimination of particular inputs or components of the model. Critical evaluation and reduction of the size of the model can help in preventing the model from becoming so large and unwieldy that it is no longer practical. Finally, sensitivity analysis can be used to help develop a ‘‘comfort level’’ with a particular model.

2.4 Model Conditional Analysis

Sensitivity analysis can also be used for conditional analysis of a model. Conditional analysis features “what-if” scenario analysis of a model and can focus on identification of factors contributing to extreme output responses and risks. In “what-if” scenario analysis, specific goals with respect to potential risk management can be modeled. Sensitivity analysis provides a tool to evaluate how these goals can be achieved by identifying key inputs and model assumptions contributing most to the predefined scenario. Through this approach, the analysis can be framed in a way that is more responsive to the public’s concerns and interests, thereby facilitating public review of the analysis. In addition, sensitivity analysis can provide explicit insight into the combination of key values and/or ranges of inputs that lead to the best, or worst, outcomes.

3. SELECTED SENSITIVITY ANALYSIS METHODS

There are different ways of classifying sensitivity analysis methods. For example, these methods may be broadly classified as mathematical, statistical (or probabilistic), and graphical (Frey and Patil, 2002). Alternatively, methods can be classified as screening, local, and global. Screening methods are typically used to make a preliminary identification of the most sensitive model inputs. However, such methods are often relatively simple and may not be robust to key model characteristics such as nonlinearity, thresholds, and interactions. Local sensitivity analysis focuses on relatively small perturbations near a fixed point in the model domain. For small perturbations of the inputs, a linear approximation may be reasonable even if the model response over a larger variation of the inputs would be nonlinear. Global sensitivity analysis methods should have the following two properties: 1) the sensitivity estimates of individual inputs take into account the effect of the range and the shape of the probability distribution for each input, and 2) the sensitivity estimates of individual inputs are obtained while all inputs vary simultaneously (Saltelli et al., 2000). In this paper, we concentrate on four methods: 1) Fourier Amplitude Sensitivity Test (FAST), 2) Response Surface Method (RSM), 3) Mutual Information Index (MII), and 4) the methods of Sobol’.

3.1 Fourier Amplitude Sensitivity Test (FAST)

FAST can identify the contribution of individual inputs to the expected value of the output variance (Cukier et al., 1978). FAST does not assume a specific functional relationship such as linearity or monotonocity in the model structure, and thus works for both monotonic and non-monotonic models (Saltelli et al., 2000). The effect of only one input or the effect of all inputs varying together can be assessed by FAST. FAST is a pattern search method that selects points in the input domain, and it is known to be faster than the Monte Carlo method (McRae et al., 1982). The classical FAST method is not efficient in addressing higher-order interaction terms (Saltelli and Bolado, 1998); however, the extended FAST method developed by Saltelli et al. (1999) can address higher order interactions between the inputs. FAST is used to estimate the ratio of the contribution of each input to the output variance with respect to the total variance of the output as the first order sensitivity index. This index can be used to rank the inputs (Saltelli et al., 2000). Because FAST can allow arbitrarily large variations in input parameters, the effect of extreme events can be analyzed (e.g., Lu and Mohanty, 2001; Helton, 1993). The evaluation of sensitivity estimates can be carried out independently for each factor using just a single set of simulations (Saltelli et al., 2000). As a drawback in application of FAST, it suffers from computational complexity for a large number of inputs (Saltelli and Bolado, 1998). FAST presents sensitivity in terms of the contribution of each input to the total output variance. The percentage contribution of each input to the total output variance can be estimated by normalizing the FAST indices for each input. FAST can provide: first-order indices, higher-order indices, and total indices. Model inputs can be ranked using the relative magnitude of sensitivity indices.

3.2 Response Surface Method (RSM)

The primary objective of the RSM is to develop a simplified version of the original model so that it is possible to retain the key characteristics of the model and to shorten the amount of time required to predict the output for a given set of inputs. RSM is typically applied to large models so that statistical methods that require multiple model evaluations can be applied. RSM is often used as a step prior to application of techniques that require many model evaluations, such as Monte Carlo simulation. A Response Surface (RS) can be linear or nonlinear, and is typically classified as first-order or second-order methods (Myers and Montgomery, 1995). For nonlinear response surfaces, interaction terms between inputs are considered. The number of inputs included in a RS and the type of RS structure required affect the amount of time and effort needed to develop a RS. It is often beneficial to limit the inputs that are included in the RS to those that are identified as most important using a screening sensitivity analysis method, such as NRSA. A typical approach to RS development is to use a least-squares regression method to fit a standardized first or second order equation to the dataset including the output values from a model and sampled values from probability distributions of model inputs. The precision and accuracy of the RS can then be evaluated by comparing the prediction of the RS with those of the original model for the same values of the model input. Because the RS is calibrated to data generated from the original model, the valid domain of applicability of the RS model will be limited to the range of values used to generate the calibration dataset. Most RS studies are based on a fewer inputs than the original model. Therefore, the effect of all original inputs on the sensitivities cannot be evaluated in RSM. If there are a large number of inputs, the RSM can be very complex.

3.3 Mutual Information Index (MII)

The objective of the Mutual Information Index (MII) sensitivity analysis method is to produce a measure of the information about the output that is provided by a particular input. The sensitivity measure is calculated based upon conditional probabilistic analysis. The magnitude of the measure can be compared for different inputs to determine which inputs provide the most information with respect to the output. MII is a computationally intensive method that takes into account the joint effects of variation in all inputs with respect to the output. MII is typically used for models with dichotomous outputs; but it can also be used for outputs that are continuous (Critchfield and Willard, 1986). The mutual information is a more direct measure of the probabilistic relationship of two random variables than other measures such as correlation coefficients (Jelinek, 1970). Calculation of the MII requires iterative application of Monte Carlo techniques that may lead to computational complexity, and thus make practical application difficult (Merz et al., 1992). Because of the simplifying approximations that may be used in MII, the robustness of ranking based on the sensitivity measure is difficult to evaluate. The mutual information between two random variables is the amount of information about a variable that is provided by the other variable (Jelinek, 1970). The average MII for each input (I_{XY}) is calculated based on the PDF of the input and on the overall and conditional confidence in the output. The amount of information about a variable that is provided by the variable itself is measured in terms of the "average self-information" (I_{YY}) of that variable. For the purpose of sensitivity analysis, a normalized measure of the MII (S_{XY}) is used which is the ratio of I_{XY} and I_{YY} (Jelinek, 1970). Application of MII involves three general steps (Critchfield and Willards, 1986): 1) generating an overall confidence measure of the output value, 2) obtaining a conditional confidence measure for a given value of an input, and 3) calculation of sensitivity indices. Sensitivity of the inputs can be evaluated based on the relative magnitude of I_{XY} and S_{XY} values estimated for each input.

3.4 Sobol' Method

Sobol' methods (Sobol, 1993; Saltelli et al., 2000) are variance-based global sensitivity analysis methods based upon "Total Sensitivity Indices" (TSI) that take into account interaction effects. The TSI of an input is defined as the sum of all the sensitivity indices involving that input. The TSI includes both the main effect as well as interaction effects (Homma and Saltelli, 1996). For example, if there are three inputs A, B and C, the TSI of input A is given by S(A) + S(AB) + S(ABC), where S(x) is the sensitivity index of x. S(A) refers to the main effect of A. S(AB) refers to the interaction effect between A and B. S(ABC) refers to the interaction effect between A, B, and C. Effort has been made to reduce the computational complexity associated with calculation of Sobol' indices. Saltelli (2002a) discusses how to make the best use of model evaluations when calculating Sobol' sensitivity indices. Sobol' method can cope with both nonlinear and non-monotonic models, and provide a truly quantitative ranking of inputs and not just a relative qualitative measure (Chan et al., 2000). The types of influence of an input that are captured by Sobol’ method include additive, nonlinear or with interactions. Furthermore, Sobol’ method can be smoothly applied to categorical variables without re-scaling. Sobol (1993) and Saltelli (2002b) describe such an implementation. Sobol’ method, in general, is computationally expensive (Pastres et. al., 1999). It can be difficult to apply Sobol’ method to models with a large number of inputs and complex model structure such as modularity.

4. SYNTHESIS AND DISCUSSION

A variety of sensitivity analysis techniques should be used to gain insights into the system model. Table 1 lists key characteristics of the selected sensitivity analysis methods. Based on the characteristics, all methods seem applicable to natural resource models. Whatever the method one uses, it is important that the framing of the analysis should be defensible for the modeler and meaningful to its users. In addition, the target of interest in sensitivity analysis should not be the model output per se, but to answer the central question for which the model was formulated. Similarly, the relevancy of the model is not the focus, but the relevancy of the model conclusions addressing the problem being solved.

Nonlinear, non-monotonic problems are often encountered in natural resource models. These problems call for a nonlinear sensitivity analysis which is independent from assumptions about the model structure. MII would require computationally intensive simulations that may be impractical unless a good response surface can be used instead of the original model. Of particular interest to sensitivity analysis practitioners in natural resource modeling are the FAST and Sobol’ sensitivity measures. These techniques can cope with nonlinear and non-monotonic models as well. They can be considered as truly quantitative for global SA for numerical experiments, e.g., the parameters can be ranked in order of their relative importance in the model.

Many of the other global sensitivity analysis methods, variance-based or not, offer at best a qualitative picture of the model sensitivity. The variance-based methods, such as correlation-ratio or importance measures, are model independent and can evaluate main effect contributions. FAST and Sobol’ are comparatively automated, and are able to compute total effect indices which allow quantitative ranking of the parameters in order of their influence (be it additive, non-linear or with interactions) on the output. These calculated indices have been termed “Total Sensitivity Indices” (TSI). TSI’s together with the first order indices should always be computed in order to investigate the predominance of lower or higher order terms. Performing the computation in this fashion helps ensure a rigorous quantitative sensitivity analysis.

Table 1. Key characteristics of selected sensitivity analysis methods (adapted from Frey et al., 2004).

Characteristic or Criteria	Sensitivity Analysis Method			
	FAST	Sobol’	RSM	MII
Simultaneous Variation	Yes	Yes	Yes	Yes
Nonlinearity	Yes	Yes	Yes	Yes
Threshold	No	No	No	No
Interaction	Yes	Yes	Yes	Yes
Qualitative vs. Quantitative Inputs	Yes	Yes	Yes	No
2D Analysis	Yes	Yes	Yes	Yes
Ease of Implementation	No	No	No	No
Quantitative Ranking of Inputs	Yes	Yes	Yes	Yes
Measure of Statistical Significance	Yes	Yes	Yes	Yes
Discrimination of Important Inputs	Yes	Yes	Yes	Yes
Robust in Practice	Yes	Yes	Yes	Yes

FAST: Fourier Amplitude Sensitivity Test
RSM: Response Surface Method
MII: Mutual Information Index

5. SUMMARY AND CONCLUSIONS

A large number of sensitivity analysis techniques are used in a wide variety of disciplines. Only four methods have been identified and discussed here for application in the natural resource discipline. The methods were selected based on a judgment that they are widely used and of potential relevance to natural resource models. Each method was characterized individually and the methods were compared on the basis of eleven criteria (Table 1). No single method is clearly superior to all others, and each method has its own key assumptions and limitations. Furthermore, each method has its own demands regarding the time and effort needed to apply the method and interpret the results; consequently, each method has strengths and limitations regarding the type of insight it can provide.

Because each sensitivity analysis method is typically based on a different assumption regarding appropriate ways of measuring sensitivity, it is quite likely that the different methods listed above may lead to different rank orderings of key inputs. Thus, a general recommendation here is to use two or more methods, preferably with dissimilar foundations, to increase confidence that the identification of key inputs is robust. Although there are theoretical arguments in favor of some methods over others, methods should be compared to evaluate whether their results differ in practice. Thus, for future work, a quantitative comparison of multiple sensitivity analysis methods applied to specific refined natural resource models is recommended. Such a comparison can provide insight regarding whether the methods, in spite of different theoretical foundations, perform similarly in practice.

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