Sensitivity analysis in presence of model uncertainty and correlated inputs

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Abstract

The first motivation of this work is to take into account model uncertainty in sensitivity analysis (SA). We present with some examples, a methodology to treat uncertainty due to a mutation of the studied model. Development of this methodology has highlighted an important problem, frequently encountered in SA: how to interpret sensitivity indices when random inputs are non-independent? This paper suggests a strategy for the problem of SA of models with non-independent random inputs. We propose a new application of the multidimensional generalization of classical sensitivity indices, resulting from group sensitivities (sensitivity of the output of the model to a group of inputs), and describe an estimation method based on Monte-Carlo simulations. Practical and theoretical applications illustrate the interest of this method.

Keywords: Global sensitivity analysis; Model uncertainty; Model mutation; Correlated inputs; Multidimensional sensitivity indices

1. Introduction

In many fields like structural reliability, behavior of thermohydraulic systems, or nuclear safety, mathematical models are used for simulation, when experiments are too expensive or even impracticable, and for prediction. In this context, sensitivity analysis (SA) tries to answer the following question: how does the output depend on its uncertain inputs? Application for SA are model calibration or model validation, and decision making process, where it is generally very useful to know which variables mostly contribute to output variability. We distinguish two classes in SA: local SA and global SA. Local SA studies how little variations of inputs around a given value change the value of the output. Global SA takes into account all the variation range of the inputs, and tries to apportion the output uncertainty to the uncertainty in the input factors. We review quickly in Section 2 a class of global SA methods based on decomposing the variance output.

The purpose of our works is to take into account a type of model uncertainty in SA, which is often encountered in practice: consider that a model, on which SA has been made is subsequently modified. In this case, is it possible to obtain information about SA of the transformed model, without doing a new complete SA, but by using instead results obtained from the original model? In Section 3, we present some useful strategies to answer this question. For some possible mutations, sensitivity indices of the transformed model can be formally related to those of original model. We also present in Section 4, a new application of group sensitivities (sensitivity of the output of the model to a group of inputs), for models with non-independent input factors.

2. Variance-based sensitivity measures

Among global SA techniques, variance-based methods are the most often used. The main idea of these methods is to express sensitivity through variance, and to evaluate how the variance of such an input or group of inputs contributes into variance of the output.
Consider the following model:

\[
f : \mathbb{R}^p \rightarrow \mathbb{R},
\]

\[
\mathbf{X} \mapsto Y = f(\mathbf{X}),
\]

(1)

where \( Y \) is the output, \( \mathbf{X} = (X_1, \ldots, X_p) \) are \( p \) independent inputs, and \( f \) is the model function, which can be analytically not known.

An indicator of the importance of an input \( X_i \) could be based on what would the variance of \( Y \) be if we fix \( X_i \) to its true value \( x_i^* \): \( \text{Var}_i(Y; \mathbf{X}) = \text{Var}(Y|X_i = x_i^*) \). This quantity is the conditional variance of \( Y \) given \( X_i = x_i^* \). But in most cases, the true value \( x_i^* \) of \( X_i \) is not known. To solve this problem, the average of this conditional variance under all possible values for \( x_i^* \), noted \( \text{Var}(Y|X_i = x_i^*) \), is studied. Using the following property:

\[
\text{Var}(Y) = \text{Var}(E(Y|X_i = x_i^*)) + E(\text{Var}(Y|X_i = x_i^*)),
\]

\[
\text{Var}(E(Y|X_i = x_i^*)) \text{ is used like an indicator of the importance of } X_i \text{ on the variance of } Y, \text{ or of the sensitivity of } Y \text{ to } X_i. \text{ This quantity, named variance of the conditional expectation and generally noted } \text{Var}(E(Y|X_i)), \text{ has an important property: the greater the importance of } X_i, \text{ the greater is } \text{Var}(E(Y|X_i)). \text{ Finally, to have a normalized indicator between 0 and 1, the used sensitivity index is defined by}
\]

\[
\frac{\text{Var}(E(Y|X_i))}{\text{Var}(Y)}.
\]

(2)

This indicator is named first-order sensitivity index by Sobol [1], correlation ratio by McKay [2], or importance measure by Ishigami and Homma [3]. It measures the main effect of \( X_i \) on the output \( Y \).

Sobol [1] has introduced this index in decomposing the model function \( f \) into summands of increasing dimensionality:

\[
f(x_1, \ldots, x_p) = f_0 + \sum_{i=1}^{p} f_i(x_i) + \sum_{1 \leq i < j \leq p} f_{ij}(x_i, x_j) + \cdots + f_{1\ldots p}(x_1, \ldots, x_p),
\]

(3)

where functions of the decomposition have two important properties: their integrals over any of its own variables are zero, and they are mutually orthogonal.

Thus, this decomposition leads to the following decomposition of the variance of \( Y \):

\[
\text{Var}(Y) = \sum_{i=1}^{p} \text{Var}_i + \sum_{1 \leq i < j \leq p} \text{Var}_{ij} + \cdots + \text{Var}_{1\ldots p},
\]

(4)

where

\[
\text{Var}_i = \text{Var}(E(Y|X_i)),
\]

\[
\text{Var}_{ij} = \text{Var}(E(Y|X_i, X_j) - E(Y|X_i)) - \text{Var}_i = \text{Var}(E(Y|X_i, X_j) - E(Y|X_i, X_j)),
\]

\[
\text{Var}_{ijk} = \text{Var}(E(Y|X_i, X_j, X_k) - E(Y|X_i, X_j, X_k)) - \text{Var}_{ij} - \text{Var}_i = \text{Var}(E(Y|X_i, X_j, X_k) - E(Y|X_i, X_j, X_k))
\]

and so on.

As all inputs are assumed to be independent, we have:

\[
V_i = V(E(Y|X_i)),
\]

\[
V_{ij} = V(E(Y|X_i, X_j)) - V_i - V_j,
\]

\[
V_{ijk} = V(E(Y|X_i, X_j, X_k)) - V_{ij} - V_{ik} - V_{jk} - V_i - V_j - V_k.
\]

From this decomposition, first-order sensitivity indices are defined by \( S_i = V_i/V(Y) \) like in (2), second-order sensitivity indices by \( S_{ij} = V_{ij}/V(Y) \), and so on. The second-order index \( S_{ij} \) expresses sensitivity of the model to the interaction between \( X_i \) and \( X_j \); the part of the variance of \( Y \) due to \( X_i \) and \( X_j \) which is not included in the individual effects of \( X_i \) and \( X_j \). It is also possible to define higher order indices.

The sum of all order indices is equal to 1, if all input variables are independent. So, in this case, index values are easy to interpret: the greater an index value, the greater is the importance of the variable or of the group of variables, that is linked to this index.

For a model with \( p \) inputs, the number of all order indices is \( 2^p - 1 \). As this number can be very important when \( p \) increases, total sensitivity indices have been introduced by Homma and Saltelli in [4]. For an input \( X_i \), the total sensitivity index \( T_{Si} \) is defined as the sum of all indices relating to \( X_i \) (first and higher order). For example, for a model with \( p = 3 \) inputs, \( T_{Si} = S_1 + S_{12} + S_{13} + S_{123} \).

One method of estimation of these indices is introduced by Sobol [1], using Monte-Carlo simulations. Saltelli extends this method for a best use of model evaluations, and also for lower cost [5]. Another method, named Fourier amplitude sensitivity test (FAST) is also defined by Cukier et al. [6] and Schaibly and Shuler [7], and extended for total indices by Saltelli et al. [8].

For more information on variance-based sensitivity measures, refer to [9].

3. Impact of model uncertainty on sensitivity analysis

Assume that a SA have been made on a model \( M : Y = f(X_1, \ldots, X_p) \), where the \( p \) input variables \( X_i \) are independent. Let us suppose that new informations about the model, new measurements, or even changes in the modelized process, oblige us to consider a new model \( M_{mut} \), that is also a mutation of the original model \( M \). Let us present some mutations, for which interesting results have been obtained. In the first one, a random variable is fixed to a given value. In the second one, we consider that we have made two sensitivity analyses on two models, and that we decide to study the sum of this two models.

3.1. A random input becomes deterministic

Suppose that a variable \( X_i \) from a given model \( Y = f(X_1, \ldots, X_p) \) is fixed to \( z \) (in practice we have most of the time \( z = E[X_i] \), but not necessarily). Is it possible to compute the new sensitivity indices of the mutated model...
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