Sensitivity Analysis in presence of model uncertainty and correlated inputs

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Abstract: First motivation of this work is to take into account model uncertainty in sensitivity analysis. So, we present in a first part, with some cases, an outline of the methodology used to treat uncertainty due to a mutation of the studied model. Development of this methodology have highlighted an important problem, frequently encoutered in sensitivity analysis: how to interpret sensitivity indices when model random inputs are non-independent? Also, we present a method to solve this problem, which introduce multidimensional sensitivity indices. Practical and theoretical applications will illustrate interest of this method.

1. INTRODUCTION

In many fields like reliability of mechanical structures, behavior of thermohydraulic systems, or nuclear safety, mathematical models are used, for simulation, when experiments are too expensive or even impracticable (nuclear accident), and for prediction.
In this context, sensitivity analysis is often used for model calibration or model validation, and to find which variables mostly contribute to output variability. In this paper, we consider global sensitivity analysis, like named in [3], based on the study of the variances of model variables. Those methods consist in the computation of sensitivity indices, which apportion the sensitivity of model output variance to model inputs. For a model

$$Y = f(X_1, ..., X_p),$$

first order sensitivity indices are defined by

$$S_i = \frac{V(E[Y|X_i])}{V(Y)}, \tag{1}$$

and express the part of variance of model output Y due to model input X_i. Higher order indices are also defined, to express effect of input interactions and total indices for total effect of one input. An important property, which enables us to easily interpret sensitivity indices values, is that the sum of all these indice is equal to 1, when inputs are independent (for more details on this property, the reader is referred to [5]). Methods of estimation of those indices are introduced by Cukier (FAST [1], [4]), Sobol [5], McKay [2], among others. We will use Sobol

method for numerical experiments.
The purpose of our works is to take into account a particular characterization of model uncertainty in sensitivity analysis. First of all, let us present this problem, often encountered in practice: consider that a model, on which sensitivity analyse have been made, undergoes a transformation, or, in other words, a mutation. In this case, is it possible to obtain information about sensitivity analysis of the mutated model, without doing a new complete analysis, but by using sensitivity results on the original model? In the first part, we will present an outline of the methodology which we used to answer to this question. For some possible mutations, we will mathematically relate sensitivity indices of original model with those of mutated model. Following nature of the mutation, some assumptions are necessary, and which one is most often met, is independence of the model inputs. As this last assumption is sometimes difficult to justify in practice, and as usual sensitivity indices (1) aren't meaningful when inputs are non-independent, we will present in a second part a new method of sensitivity analysis for those models.

2. IMPACT OF MODEL UNCERTAINTY ON SENSITIVITY ANALYSIS

Assume that a sensitivity analysis have been made on a model $M : Y = f(X_1, ..., X_p)$, where the n inputs variables X_i are independent. Let us suppose that new informations about the model, new measurements, or even changes in the modelled process, oblige us to consider a new model M_{mut}, that is also a mutation of the original model M. Rather than to make an exhaustive list of all possible mutations, let us present only some usefull mutations, for which interesting results have been obtained.
Firstly, consider a model $M : Y = f_1(X_1) + f_2(X_2, ..., X_p)$, where $(X_1, ..., X_p)$ are independent random variables, and suppose that M undergoes a mutation, and is also transformed in a new model M_{mut} where X_1 is fixed to its mean $\mu_1 = E[X_1]$. Thus, this new model is $Y^m = f_1(\mu_1) + f_2(X_2, ..., X_p)$. Writing definition of sensitivity indices, we show that M_{mut} sensitivity indices (S^m) can be express from sensitivity indices (S) of M by:

$$S^m = S \times \frac{V(Y)}{V(Y^m)} \quad \text{for first and higher order sensitivity indices.}$$

and by:

$$S_T^m = 1 - (1 - S_T) \times \frac{V(Y)}{V(Y^m)} \quad \text{for all total sensitivity indices.}$$

Of course, all indices relating to variable X_1 disappear.
Let us consider now inverse case, which can be view as introduction of noise in the model, and which consist to consider a deterministic parameter like a random variable. So the model $M : Y = f_1(\mu) + f_2(X_1, ..., X_p)$ is mutated in a model $M_{mut} : Y^m = f_1(X_{p+1}) + f_2(X_1, ..., X_p)$. In this case, sensitivity indices of M_{mut}, are given by those of M multiplied by $V(Y)$ and divided by $V(f_1(X_{p+1})) + V(Y)$. For the new variable, only first order indice are non zero, and is given by

$$\frac{V(f_1(X_{p+1}))}{V(f_1(X_{p+1})) + V(Y)}.$$

For the same mutation carried out on the model $M : Y = f_1(\mu) \times f_2(X_1, ..., X_p)$, sensitivity indices of M_{mut} can be obtain multiplying indices of M by

$$\frac{V(Y)}{V(Y^m)} \times \left(\frac{E[f_1(X_{p+1})]}{f_1(\mu)} \right)^2 .$$

Now, if we consider the new variable X_{p+1} as dependent from the others variables, we are again confronted with the problem of sensitivity analysis for model with dependent inputs previously evoked. Also, we don't know to deduce sensitivity indices of the mutated model from the knowledge of the M model.

Let us finally present an other type of mutation. Assume that two analysis have been made on two models $M_1 : Y_1 = f_1(X_1, ..., X_p)$ and $M_2 : Y_2 = f_2(X_{p+1}, ..., X_{p+q})$, and also that sensitivity indices S^1 for M_1 and S^2 for M_2 have been computed. We suppose that inputs variables of the two models are different and independent. Let us create a new model M_{mut} : $Y^m = Y_1 + Y_2$. Sensitivity indices of M_{mut} are obtained by multiplying

$$\text{those of } M_1 \text{ by } \frac{V(Y_1)}{V(Y_1) + V(Y_2)} \text{ and those of } M_2 \text{ by } \frac{V(Y_2)}{V(Y_1) + V(Y_2)}.$$

All sensitivity indices, relative to interaction between M_1 variables and M_2 ones are equal to zero. If we suppose that there are dependences between variables of the two models, we are afresh confronted with the same problem of sensitivity analysis for dependant or correlated inputs.

To conclude, if an original model, on which sensitivity analysis have been made, is transformed, it's possible to deduce sensitivity indices of the mutated model, without starting again heavy calculation of Monte Carlo, in a given number of cases. Those cases are principally deletion of variables or introduction of new independent variables. On the other hand, introduction of dependent variables, or even of existing variables poses the problem of sensitivity analysis with dependent inputs, for which we propose a new method.

3. SENSITIVITY ANALYSIS FOR MODEL WITH DEPENDENT OR CORRELATED INPUTS

Highlighted in previous section, the problem of sensitivity analysis for model with dependent inputs is a real one, because naturally frequently met in practice.

This problem concern the interpretation of sensitivity indices values. When inputs are independent, I.M.Sobol demonstrates that the sum of all sensitivity indices is equal to 1. Effectively, in Sobol's decomposition of model function, all term are mutually orthogonal if inputs are independent, and so we can obtain a variance decomposition of model output. Dividing this decomposition by output variance, we obtain exactly that the sum of all order indices is equal to 1. If we don't assume that the inputs are independent, the terms of model function decomposition are not orthogonal, and so it appears a new term in the variance decomposition. That's this term which implies that the sum of all order sensitivity indices is not equal to 1. We can give the following interpretation to this : when we study sensitivity of one input, which is correlated with another one, we study too sensitivity of this last. Effectively, variabilities of two correlated variables are link, and so when we quantify sensitivity to one of this two variables, we quantify

too a part of sensitivity to the other variable. And so, in sensitivity indices of the two variables, the same information is taken into account several times, and sum of all indices is thus greatest than 1.
Natural idea is also coming: to define multidimensional sensitivity indices for groups of correlated variables.

3.1. Multidimensional sensitivity analysis

Consider the model

$$Y = f(X_1, ..., X_p),$$

where

$$(X_1, ..., X_p) = (\underbrace{X_1}_{\mathbb{X}_1}, ..., \underbrace{X_i}_{\mathbb{X}_i}, \underbrace{X_{i+1}, ..., X_{i+k_1}}_{\mathbb{X}_{i+1}}, \underbrace{X_{i+k_1+1}, ..., X_{i+k_2}}_{\mathbb{X}_{i+2}}, ..., \underbrace{X_{i+k_{l-1}+1}, ..., X_p}_{\mathbb{X}_{i+l}})$$

$(X_1, ..., X_i) = (\mathbb{X}_1, ..., \mathbb{X}_i)$ are independent inputs, and $(\mathbb{X}_{i+1}, ..., \mathbb{X}_{i+l})$ are l groups of intra-dependent or intra-correlated inputs ($\mathbb{X}_i$ are independent of $\mathbb{X}_j$, for all $1 \leq i, j \leq l$).
We wrote monodimensional non independent variables $(X_1, ..., X_p)$ like multidimensional independent variables $(\mathbb{X}_1, ..., \mathbb{X}_{i+l})$.
Thus, we define first order sensitivity indices

$$S_j = \frac{V(E[Y|\mathbb{X}_j])}{V(Y)} \quad \forall j \in [1, i+l]$$

To connect this to monodimensional variables, if $j \in [1, ..., i]$, we have well define the same indice:

$$S_j = \frac{V(E[Y|\mathbb{X}_j])}{V(Y)} = \frac{V(E[Y|X_j])}{V(Y)} \tag{2}$$

and if $j \in [i+1, ..., i+l]$, for example $j = i+2$:

$$S_j = S_{\{i+k_1+1,...,i+k_2\}} = \frac{V(E[Y|X_{i+k_1+1}, ..., X_{i+k_2}])}{V(Y)} \tag{3}$$

Now, like in classical analysis, we can also define higher order indices and total sensitivity indices. Second order indices are given by

$$S_{jk} = \frac{V(E[Y|\mathbb{X}_j, \mathbb{X}_k] - E[Y|\mathbb{X}_j] - E[Y|\mathbb{X}_k])}{V(Y)},$$

and so on for higher order indices. And finally, total order indices are defined by :

$$S_{T_j} = \sum_{k\#j} S_k,$$

where $\#j$ represent all subsets of $\{1, ..., i+l\}$ which include j.
It's very important to note that if all input variables are independent, those sensitivity indices are clearly the same than (1). And so, multidimensional sensitivity indices can well be interpreted like a generalization of usual sensitivity indices (1).

3.2. Numerical estimation

Like in classical analysis (Sobol), Monte-Carlo estimations are possible.
We estimate mean and variance of Y by :

$$\hat{f}_0 = \frac{1}{N}\sum_{k=1}^{N} f(\mathbf{x}_1^k, ..., \mathbf{x}_{i+l}^k) \qquad \hat{D} = -\hat{f}_0^{\ 2} + \frac{1}{N}\sum_{k=1}^{N} f^2(\mathbf{x}_1^k, ..., \mathbf{x}_{i+l}^k),$$

and first order indice by $\hat{S}_j = \frac{\hat{D}_j}{\hat{D}}$ with :

$$\hat{D}_j = \frac{1}{N}\sum_{k=1}^{N} f(\mathbf{x}_1^k, ..., \mathbf{x}_{j-1}^k, \mathbf{x}_j^k, \mathbf{x}_{j+1}^k, ..., \mathbf{x}_{i+l}^k) f(\mathbf{x}_1^k, ..., \mathbf{x}_{j-1}^k, \underline{\mathbf{x}}_j^k, \mathbf{x}_{j+1}^k, ..., \mathbf{x}_{i+l}^k) - \hat{f}_0^2,$$

where $(\mathbf{x}_1^k, ..., \mathbf{x}_{i+l}^k)_{k=1,N}$ and $(\underline{\mathbf{x}}_1^k, ..., \underline{\mathbf{x}}_{i+l}^k)_{k=1,N}$ are two independent sets of N (multidimensional) inputs simulations. Equivalent estimations for higher order and total indices exist.

3.3. Application in nuclear field - epithermal indice

Study presented here is a sensitivity analysis of a model, which compute an epithermal indice for a given nuclear reactor. The epithermal indice is defined by the value of the neutron epithermal flow divided by the neutron thermal flow. This indice is useful in studies of nuclear reactor vessel dosimetry.
This model is made of 4 inputs, of which two are correlated:

$$\begin{aligned}
\text{resonance integral of Co59} &: \quad X_1 \sim \mathcal{N}(72, 7.2^2) \\
\text{factor Fcd} &: \quad X_2 \sim \mathcal{N}(\log(1.01989), 0.0147051^2) \\
\text{activity of the dosimeter Co59 "nu"} &: \quad X_3 \sim \mathcal{N}(4.703 \times 10^7, 1147732^2) \\
\text{activity of the dosimeter Co59 under Cadmium} &: \quad X_4 \sim \mathcal{N}(2.522 \times 10^7, 615368^2) \\
\text{with correlation coefficient} & \quad\ \ \rho_{X_3X_4} = 0.85,
\end{aligned}$$

one output Y : epithermal indice, and one function which links inputs and output:

$$Y = \frac{\exp X_2(1.008843 - 0.02114316X_1 + 9.858080.10^{-5}X_1^2 + 1.931988.10^{-8}X_4)}{(1 - \exp X_2\frac{X_4}{X_3})(-0.00575077 + 3.73935.10^{-8}X_3)}.$$

Like explicited previously, as two inputs are correlated, it's useless to compute usual sensitivity indices, because results will not be meaningful. We thus carried out a multidimensionnal sensitivity analysis. Numerical experiments have been made repeating all indices computations 20 times, with $N = 20000$ Monte-Carlo iterations. Mean of these 20 estimations, represented on figure 1, are the following:

$$S_1 \simeq 0.85 \quad S_2 \simeq 0.09 \quad S_{\{3,4\}} \simeq 0.07$$
$$S_{12} \simeq S_{1\{3,4\}} \simeq S_{2\{3,4\}} \simeq S_{12\{3,4\}} \simeq 0$$

where $S_{\{3,4\}}$ are the first order sensitivity indices of the multidimensional variable $\{X_3, X_4\}$.
Multidimensional analysis allows us to conclude that this model is sensitive essentially to input

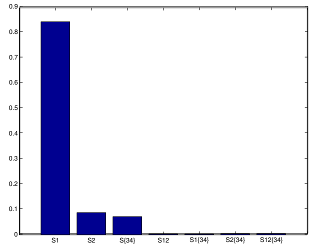

Figure 1. Sensitivity indices of epithermal indice model

X_1 (*resonance integral of Co59*), and that others variables are less significant. But in this application, the interest of our method is not very well exhibit. Effectively, as X_1 and X_2 are independent from the other variables, we can apply classical sensitivity analysis and find the same value for S_1 and S_2. And also, as the sum of this two indices are equal to 0.94, we can deduce that the other variables and all the interaction with them, have only small importance. We will present a theoretical application, which emphasizes more multidimensional sensitivity analysis.

3.4. Theoretical application

Consider the model

$$Y = aX_1X_2 + bX_3X_4 + cX_5X_6,$$

where $X_i \sim \mathcal{N}(0,1)$, for $i = 1$ to 6, and where X_3 and X_4 are correlated ($\rho_{X_3,X_4} = \rho_1$), like X_5 and X_6 ($\rho_{X_5,X_6} = \rho_2$). Sensitivity indices are the following:

$$\begin{aligned} S_{12} &= \frac{a^2}{a^2 + b^2(1+\rho_1)^2 + c^2(1+\rho_2)^2} \\ S_{\{3,4\}} &= \frac{b^2(1+\rho_1)^2}{a^2 + b^2(1+\rho_1)^2 + c^2(1+\rho_2)^2} \\ S_{\{5,6\}} &= \frac{c^2(1+\rho_2)^2}{a^2 + b^2(1+\rho_1)^2 + c^2(1+\rho_2)^2} \end{aligned}$$

and all the other indices are equal to 0. We constate that the value of the numerator of the interaction sensitivity indice S_{12} is a function of the coefficient a. The values of numerators of the non zero sensitivity indices $S_{\{3,4\}}$ and $S_{\{5,6\}}$ are function of the model coefficients b and c, but too of the correlation coefficient ρ_1 or ρ_2. To illustrate this, let us present some numerical values of those indices, for different values of the coefficients of the model (a, b and c) and the correlation coefficients.

situation	a	b	c	ρ_1	ρ_2	S_{12}	$S_{\{3,4\}}$	$S_{\{5,6\}}$
(i)	1	1	1	0.8	0.8	0.2336	0.3832	0.3832
(ii)	3	1	1	0.8	0.8	0.7329	0.1336	0.1336
(iii)	1	1	3	0.8	0.8	0.0575	0.0943	0.8483
(iv)	1	1	1	0.8	0.3	0.2881	0.4397	0.2922
(v)	1	1	3	0.8	0.3	0.0803	0.1317	0.7880
(vi)	1	1	3	0.3	0.8	0.0593	0.0647	0.8760

First of all, let us underline that as X_1 and X_2 are independent variables, indices S_1, S_2, and S_{12} are usual sensitivity indices, and can also be computed without our multidimensional method.
In the situation (ii), as X_1 and X_2 are independent variables, usual sensitivity indices allows us to conclude that variance of Y is essentially (73%) due to interaction between X_1 and X_2. But in the others situations, when X_1 and X_2 are less important, we need multidimensional sensitivity indices to apportions effect to the two couple (X_3, X_4) and (X_5, X_6). These multidimensionnal indices allow us to know that couple (X_3, X_4) and (X_5, X_6) have the same importance in the situation (i), and that (X_5, X_6) is the most important in situation (iii). Effectively, in situation (i) couples (X_3, X_4) and (X_5, X_6) are symmetric in the model, and so they have same importance. In (iii) a coefficient equal to 3 is multiplying the product X_5X_6, that's why the couple (X_5, X_6) is most important than (X_3, X_4).
Situations (iv), (v) and (vi) illustrate that indices $S_{\{3,4\}}$ and $S_{\{5,6\}}$ are function to the correlation (S_{12} is too function to the correlation, but it's due to its denominator, which is the variance of Y). As couples (X_3, X_4) and (X_5, X_6) are in the model in a product form: X_3X_4 and X_5X_6, greater is the correlation, greater is the importance of the couple, and so greater is the value of the sensitivity indices. In (iv) the correlation of (X_3, X_4) is greater than correlation of (X_5, X_6), and so $S_{\{3,4\}}$ is greater than $S_{\{5,6\}}$. In situations (v) and (vi), we can see the same behaviour.

4. CONCLUSION AND FUTURE WORK

We have presented in this paper two works : the first concern integration of a view point of model uncertainty in sensitivity analysis, which we interpret like a model mutation. We drew up an outline of the employed methodology, which consists in a listing of possible mutations, for each one which we examine the impact on the computing of sensitivity indices. Second work introduces a new method which allows to compute useful and comprehensible sensitivity indices for a model with non-independent inputs. Practical and theoretical illustrations of interest of this method have been presented.
Further applications and developments are envisaged, in particular when there are many model inputs.

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