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## 1. GENERAL REMARKS

Mathematical models play an increasingly important role to simulate, study and predict future outcomes in every field of science. These models, generally, involve a large set of input variables (whose values are often imprecisely known). With problems of this type, it is important to understand the relationships between the input variables and the output. Sensitivity analysis (SA) allows one to study these relationships and identify the most significant factors or variables affecting the results of the model. The global SA methods can also be used for model calibration, model validation, decision making process, i.e., any process where it is useful to know which are the variables that mostly contribute to the output variability.

Let define the model  $f: \Re^p \to \Re$  and Y = f(X) that can also be considered as a "black box" where Y is the output of model and  $X = X_1, \ldots, X_p$  are p-independent inputs. The effect of the variance of an input or a group of input parameters contributes to the output variance of f are described using the so-called Sobol's indexes. For a model with p inputs, the number of Sobol's indices is  $2^p - 1$ ; leading to an intractable number of indices as p increases. Thus, to express the overall output sensitivity to an input  $X_i$ , the total sensitivity index,  $S_{T_i} = S_i + \sum_{j \neq i} S_{ij} + \sum_{j \neq i, k \neq i, j < k} S_{ijk} + \ldots$ , can be used [1]. Recent global SA techniques take into account the entire range of variation of the inputs and aim to apportion the whole output uncertainty to the input factor uncertainties (see e.g [4]).

Working in a standard normal space (obtained by means of e.g. the Nataf transformation), where the factors  $x_1, \ldots, x_p$  are independent standard normal random variables, it has been shown [5] that the total sensitivity indexes has the following upper bound:

(1) 
$$S_i^{tot} \le \frac{\nu_i}{D} = \frac{\int_{H^p} \left(\frac{\partial f}{\partial x_i}\right)^2 d\mathbf{x}}{D}$$

where D is the total variance of f,  $\nu_i$  are functions similar to the Morris importance measures [2] and  $H^n$  represents the standard normal space of dimension p. The estimation of  $\nu_i$  can be performed by simple Monte Carlo (independent random samples) simulation.

The major drawback of this approach is that it may be CPU time consuming, mainly because of the sampling method. In case the total sensitivity is evaluated for all p components, the cost to estimate p total sensitivity indices is  $N_t = N(p+1)$ . It is well known that, for complex computer models, an accurate estimation of these indexes by the simple Monte Carlo method requires N > 1000. In complex industrial applications, this approach is intractable due to the CPU time cost of one model evaluation and the possible large number of input parameters.

## 2. PROPOSED APPROACH

The aim of this paper is to present an efficient Monte Carlo based approach for the estimation of the upper bound of  $S_i^{tot}$  where  $n \ll N$  samples are required to estimate the (upper)

bound of each index. The main idea is to estimate the gradient components of a generic function by means of a Monte Carlo procedure along the points sampled from a Markov-chain. It has been shown [3] that adopting an orthogonal linear transformation it is possible to identify a new coordinate system where a relatively small subset of the variables contributes significantly to the gradient. Working in this transformed space only few samples, i.e. much less than the dimensionality of the problem, are required in order to estimate the gradient components,  $\frac{\partial f}{\partial x_i}$ . The ideal rotation requires the knowledge of the gradient at the same point; however an approximate rotation can be performed by adopting, for instance, the values of the gradient evaluated in the previous point of the Markov chain. It is, nonetheless, correct to state, that in most applications only a small subset of parameters is likely to cause most of the response variability, whereas a large part of parameters will have an insignificant effect on the solution, i.e. the gradient has few dominant components.

At each point of the Markov chain, the gradient is not determined directly, as it is the case for finite difference procedures or direct differentiation procedures, but by random sampling in the close neighbourhood of the current chain point,  $\mathbf{x} = \tilde{\mathbf{x}}$ . The following function difference,  $\mathbf{b}^{(j)}(\tilde{\mathbf{x}}) = f(\tilde{\mathbf{x}} + \gamma \cdot \mathbf{R}^{(j)}) - f(\tilde{\mathbf{x}})$  is then computed from simulation where the parameter  $\gamma > 0$  controls the width of scatter points  $\mathbf{x}^{(j)}$  around the reference point  $\tilde{\mathbf{x}}$  and R is a vector full of i.i.d. standard normal random variables. The components of the derivative at the point  $\tilde{\mathbf{x}}$  are:

(2) 
$$d_k^{(j)}(\tilde{\boldsymbol{x}}) = \left. \frac{\partial f(\boldsymbol{x})}{\partial x_k} \right|_{\boldsymbol{x} = \tilde{\boldsymbol{x}}} \approx \frac{b_k^{(j)}(\tilde{\boldsymbol{x}})}{\gamma \cdot R_h^{(j)}}$$

The most important gradient components can be estimated from certain statistics as shown in Ref [3]. Finally the following estimators can be used to calculate the functional  $\nu_i$  as well as the Morris importance measures,  $\mu_i$ :

(3) 
$$\nu_i = \int_{H^p} \left( \frac{\partial f(\boldsymbol{x})}{\partial x_i} \right)^2 dx \approx \frac{1}{N_{chain}} \sum_j \left( \frac{b_k^{(j)}(\tilde{\boldsymbol{x}})}{\gamma \cdot R_k^{(j)}} \right)^2; \qquad \mu_i \approx \frac{1}{N_{chain}} \sum_j \left| \frac{b_k^{(j)}(\tilde{\boldsymbol{x}})}{\gamma \cdot R_k^{(j)}} \right|$$

where  $N_{chain}$  represents the length of the Markov chain with the points distributed according the multivariate normal distribution.

In conclusion, this approach allows a significant reduction of the computational efforts required to perform the global SA especially for applications involving a high number of variables.

## 2. REFERENCES

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