SOBOL' INDICES FOR PROBLEMS DEFINED IN NON-RECTANGULAR DOMAINS

S. Kucherenko, O.V. Klymenko, N. Shah
Imperial College London, London, SW7 2AZ, UK
s.kucherenko@imperial.ac.uk

Uncertainty and sensitivity analysis has been recognized as an essential part of model applications. Global sensitivity analysis (GSA) is used to identify key parameters whose uncertainty most affects the output. This information can be used to rank variables, fix or eliminate unessential variables and thus decrease problem dimensionality. Among different approaches to GSA variance-based Sobol sensitivity indices (SI) are most frequently used in practice owing to their efficiency and ease of interpretation [1-3]. Most existing techniques for GSA were designed under the hypothesis that model inputs are independent. However, in many cases there are dependences among inputs, which may have significant impact on the results. Such dependences in a form of correlations have been considered in the generalised Sobol GSA framework developed by Kucherenko *et al,* [4]. However, there is an even wider class of models involving inequality constraints (which naturally leads to the term constrained GSA or cGSA) imposing structural dependences between model variables. This implies that the parameter space may no longer be considered to be an *n*-dimensional hypercube which is the case in existing GSA methods, but may assume any shape depending on the number and nature of constraints. This class of problems encompasses a wide range of situations encountered in the natural sciences, engineering, design, economics and finances where model variables are subject to certain limitations imposed e.g. by conservation laws, geometry, costs, quality constraints etc.

The development of efficient computational methods for cGSA is challenging because of potentially arbitrary shape of the feasible domain of model variables variation, thus requiring the development of special Monte Carlo or quasi-Monte Carlo sampling techniques and methods for computing sensitivity indices. We developed a novel method for estimation of Sobol' SI for models $f\left(x_1,...,x_n\right)$ defined in a non-rectangular domain Ω^n. Consider an arbitrary subset of the variables $y=\left(x_{i_1},...,x_{i_s}\right)$, $1\le s<n$ and a complementary subset $z=\left(x_{i_{s+1}},...,x_{i_n}\right)$, so that $\left(x_1,...,x_n\right)=(y,z)$. Then formulas for the main effect and total Sobol' SI have the following form:

$$S_y=\frac{1}{D}\left[\int_{\Omega^n} f(y',z')p^{\Omega}(y',z')dy'dz'\left[\int_{\Omega^{n-s}}\frac{f(y',z)}{p^{\Omega}(y')}p^{\Omega}(y',z)dz-\int_{\Omega^n} f(y,z)p^{\Omega}(y,z)dydz\right]\right],$$

$$S_y^T=\frac{1}{2D}\int_{\Omega^n}\int_{\Omega^s}[f(y,z)-f(y',z)]^2 p^{\Omega}(y,z)\frac{p^{\Omega}(y',z)}{p^{\Omega}(z)}dydy'dz.$$

Here $p^{\Omega}(y,z)$ is a joint probability distribution and $p^{\Omega}(y)$ is a marginal distribution. Both distributions are defined in Ω^n. We propose two methods for estimation Sobol' SI: 1) quadrature integration method which may be very efficient for problems of low and medium dimensionality; 2) MC/QMC estimators based on the acceptance-rejection sampling method. A few model test functions with constraints are considered for which we found analytical solutions. These solutions are used as benchmark test for verifying for the quadrature and MC and QMC integrations methods. One of the models is the K-function $K=\sum_{i=1}^{n}(-1)^i\prod_{j=1}^{i}x_j$, where variables x_j, $j=1,...,n$, $n=4$ are independent uniformly distributed random variables in [0, 1]. We consider four different cases for domain definitions. The first one is an unconstrained problem ($x\in H^n$). In the other three cases the unit hypercube is divided by a hyperplane into two parts one of which is the permissible region for the problem variables x_j, $j=1,...,n$. The constraints are as follows:

$$I_1 : x_1 + x_2 \le 1,$$
$$I_2 : x_3 + x_4 \le 1,$$
$$I_3 : x_1 + x_3 \le 1.$$

These constraints can be represented using the following indicator functions: $I_1 = U(1 - x_1 - x_2)$, $I_2 = U(1 - x_3 - x_4)$, $I_3 = U(1 - x_1 - x_3)$. Fig. 1 shows a schematic plot illustrating I_1 constraint in the 3D space.

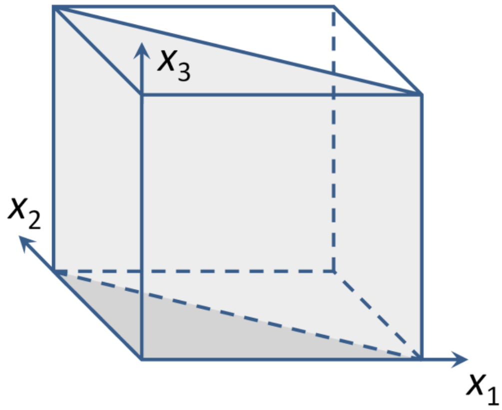

Fig. 1. Schematic representation of a permissible region for the K-function (shaded area) in the 3D case.

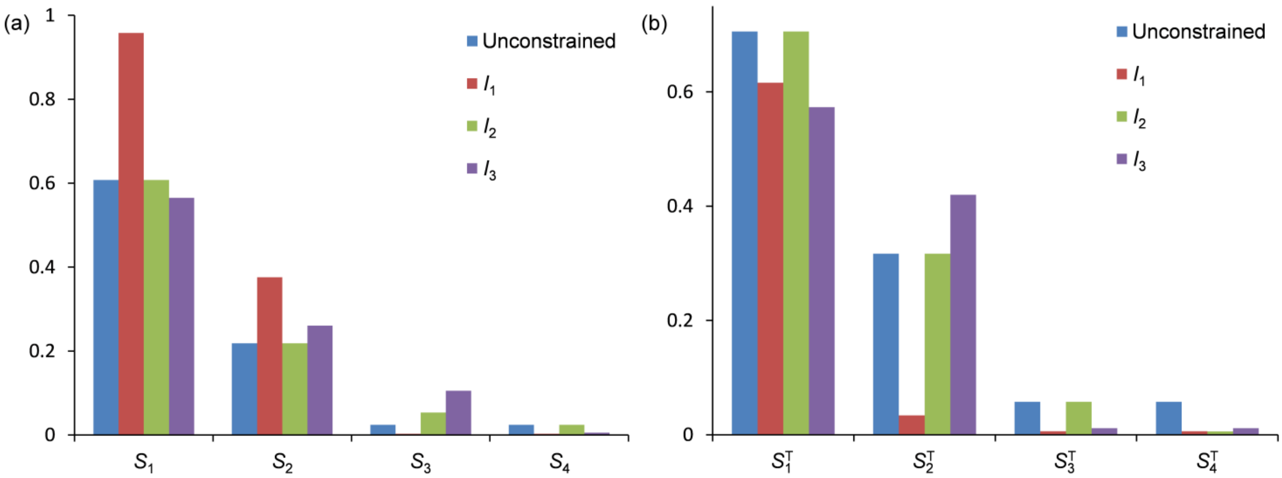

Fig. 2. (a) Main effect and (b) total sensitivity indices of the K-function in H^4 for the unconstrained and constraints cases

The values of S_i and S_i^T for all four cases are presented in Fig. 2. The method is shown to be general and efficient.

1. A. Saltelli, S. Tarantola, F. Campolongo, M. Ratto, *Sensitivity analysis in practice.* London, Wiley; 2004.
2. I. Sobol', Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. *Math Comput Simul*, 55(1–3), 271–280, 2001.
3. A. Owen, Better estimation of small Sobol' sensitivity indices. *ACM Trans on Mod and Comp Simul*, 23(11), 1-17, 2013.
4. S. Kucherenko, S. Tarantola, P. Annoni. Estimation of global sensitivity indices for models with dependent variables. *Comput. Phys. Commun*. 183, 937-946, 2012.