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Derivative based global sensitivity measures

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Abstract

We introduce new global sensitivity measures called derivative based global sensitivity measures (DGSM). We also show that there is a link between DGSM and Sobol' total sensitivity indices which makes this approach theoretically sound and general. It can be seen as the generalization of the Morris method. The computational time required for numerical evaluation of DGSM can be much lower than that for estimation of the Sobol' sensitivity indices although it is problem dependent. The efficiency of the method can be further improved by using the automatic differentiation algorithm for calculation DGSM.

Keywords: Global sensitivity analysis; Global sensitivity index; Monte Carlo method; Derivative based global sensitivity measure

1. Main text

Variance-based global sensitivity analysis (SA) methods require a large number of function evaluations to achieve acceptable convergence and can become impractical for large engineering problems. This is why a number of alternative SA techniques have been proposed. One of the most popular techniques is the screening method proposed by Morris. The revised version of the Morris method based on absolute values of elementary effects and a more effective sampling strategy, which allows a better exploration of the space of the uncertain input factors was proposed by Campolongo *et al.* [1]. The Morris method uses random sampling of points from the fixed grid (levels) for averaging elementary effects which are calculated as finite differences with the increment delta comparable with the range of uncertainty. For this reason it can not correctly account for the effects with characteristic dimensions much less than delta.

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We developed a novel approach called derivative based global sensitivity measures (DGSM). The method is based on averaging local derivatives using Monte Carlo or preferably Quasi Monte Carlo sampling methods. Our technique is much more accurate than the Morris method as the elementary effects are evaluated as strict local derivatives with small increments compared to the variable uncertainty ranges. The method also benefits from much higher convergence rate if Quasi Monte Carlo sampling methods are used. It becomes especially efficient if automatic calculation of derivatives is used.

We consider a model function $f\ \ x_1,...,x_n$ defined in the unit hypercube H^n with Lebesque measure $dx = dx_1 \cdots dx_n$. If the function f is differentiable, functionals depending on $\partial f / \partial x_i$ can be used as estimators for the influence of x_i. The Morris modified importance is an approximation of the functional $\mu_i^* = \int\limits_{H^n} \left| \frac{\partial f}{\partial x_i} \right| dx$ [1]. In [2] we suggested to use a similar functional, which we called derivative based global sensitivity measure

$$\nu_i = \int\limits_{H^n} \left(\frac{\partial f}{\partial x_i} \right)^2 dx .$$

Evidently, $\mu_i^* \le \sqrt{\nu_i}$, and $\nu_i \le C\mu_i$ if $\left| \frac{\partial f}{\partial x_i} \right| \le C$. A link between ν_i and the total sensitivity index S_i^{tot} is established:

$$S_i^{tot} \le \nu_i \big/ \ \pi^2 D \ \ ,$$

where D is the total variance of $f\ \ x_1,...,x_n$. Thus small ν_i imply small S_i^{tot}, and unessential factors x_i (that is x_i corresponding to a very small S_i^{tot}) can be detected analyzing computed values $\nu_1,...,\nu_n$. However, ranking influential factors x_i using these values can be different from that based on the global sensitivity indices.

Let $x = \ x_1,...,x_n$ be a point in H^n Consider an arbitrary subset of the variables $y = \ x_{i_1},...,x_{i_s}$, $1 \le s < n$. A derivative based criterion τ_y for groups of input variables is defined as

$$\tau_y = \sum_{p=1}^{s} \int \left(\frac{\partial f \ \ x}{\partial x_{i_p}} \right)^2 \frac{1 - 3x_{i_p} + 3x_{i_p}^2}{6} dx$$

Theorem 1 If $f\ \ x$ is linear with respect to $x_{i_1},...,x_{i_s}$, then $S_y^{tot} = \frac{\tau_y}{D}$.

Theorem 2 A general inequality holds: $S_y^{tot} \le \frac{24}{\pi^2} \frac{\tau_y}{D}$.

Proofs are given in [3]. Applications of DGSM are presented in [4].

2. References

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