Derivative based global sensitivity measures

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Abstract

The method of derivative based global sensitivity measures (DGSM) has recently become popular among practitioners. It has a strong link with the Morris screening method and Sobol' sensitivity indices and has several advantages over them. DGSM are very easy to implement and evaluate numerically. The computational time required for numerical evaluation of DGSM is generally much lower than that for estimation of Sobol' sensitivity indices. This paper presents a survey of recent advances in DGSM concerning lower and upper bounds on the values of Sobol' total sensitivity indices S_i^{tot}. Using these bounds it is possible in most cases to get a good practical estimation of the values of S_i^{tot}. Several examples are used to illustrate an application of DGSM.

Keywords: Sensitivity analysis, Sobol' indices, Morris method, Model derivatives, DGSM, Poincaré inequality

Introduction

Global sensitivity analysis (SA) offers a comprehensive approach to the model analysis. Unlike local SA, global SA methods evaluate the effect of a factor while all other factors are varied as well and thus they account for interactions between variables and do not depend on the choice of a nominal point. Reviews of different global SA methods can be found in Saltelli et al [30] and Sobol and Kucherenko [37]. The method of global sensitivity indices suggested by Sobol [33, 34], and then further developed by Homma and Saltelli [11] is one of the most efficient and popular global SA techniques. It belongs to the class of variance-based methods. These methods provide information on the importance of different subsets of input variables to the output variance. There are two types of Sobol' sensitivity indices: the main effect indices, which estimate the individual contribution of each input parameter to the output variance, and the total sensitivity indices, which measure the total contribution of a single input factor or a group of inputs. The total sensitivity indices are used to identify non-important variables which can then be fixed at their nominal values to reduce model complexity. This approach is known as "factors' fixing setting" [30]. For high-dimensional models the direct application of variance-based global SA measures can be extremely time-consuming and impractical.

A number of alternative SA techniques have been proposed. One of them is the screening method by Morris [21]. It can be regarded as global as the final measure is obtained by averaging local measures (the elementary effects). This method is considerably cheaper than the variance based methods in terms of computational time. The Morris method can be used for identifying unimportant variables. However, the Morris

method has two main drawbacks. Firstly, it 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. Secondly, it lacks the ability of the Sobol' method to provide information about main effects (contribution of individual variables to uncertainty) and it can't distinguish between low and high order interactions.

This paper presents a survey of derivative based global sensitivity measures (DGSM) and their link with Sobol' sensitivity indices. DGSM are based on averaging local derivatives using Monte Carlo or Quasi Monte Carlo sampling methods. This 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. Local derivatives are evaluated at randomly or quasi randomly selected points in the whole range of uncertainty and not at the points from a fixed grid.

The so-called alternative global sensitivity estimator defined as a normalized integral of partial derivatives was firstly introduced by Sobol and Gershman [36]. Kucherenko et al [17] introduced some other DGSM and coined the acronym DGSM. They showed that DGSM can be seen as the generalization of the Morris method [21]. Kucherenko et al [17] also established empirically the link between DGSM and Sobol' sensitivity indices. They showed that the computational cost of numerical evaluation of DGSM can be much lower than that for estimation of Sobol' sensitivity indices.

Sobol and Kucherenko [38] proved theoretically that, in the cases of uniformly and normally distributed input variables, there is a link between DGSM and the Sobol' total sensitivity index S_i^{tot} for the same input. They showed that DGSM can be used as an upper bound on total sensitivity index S_i^{tot}. Small values of DGSM imply small

S_i^{tot}, and hence unessential factors x_i. However, ranking influential factors using DGSM can be similar to that based on S_i^{tot} only for the case of linear and quasi-linear models. For highly non-linear models two rankings can be very different. They also introduced modified DGSM which can be used for both a single input and groups of inputs [39]. From DGSM, Kucherenko and Song [16] have also derived lower bounds on total sensitivity index. Lamboni et al [19] extended results of Sobol' and Kucherenko for models with input variables belonging to the general class of continuous probability distributions. In the same framework, Roustant et al [28] have defined crossed-DGSM, based on second-order derivatives of model output, in order to bound the total Sobol' indices of an interaction between two inputs.

All these DGSM measures can be applied for problems with a high number of input variables to reduce the computational time. Indeed, the numerical efficiency of the DGSM method can be improved by using the automatic differentiation algorithm for calculation DGSM as was shown in Kiparissides et al [15]. However, the number of required function evaluations still remains to be proportional to the number of inputs. This dependence can be greatly reduced using an approach based on algorithmic differentiation in the adjoint or reverse mode [9] (Variational Methods). It allows estimating all derivatives at a cost at most 4-6 times of that for evaluating the original function [13].

This paper is organised as follows: the Morris method and DGSM are firstly described in the following section. Sobol' global sensitivity indices and useful relationships are then introduced. Therefore, DGSM-based lower and uppers bounds on total Sobol' sensitivity indices for uniformly and normally distributed random variables are presented, followed by DGSM for groups of variables and their link with total Sobol' sensitivity indices. Another section presents the upper bounds results in the general case of variables with continuous probability distributions. Then, computational costs

are considered, followed by some test cases which illustrate an application of DGSM and their links with total Sobol' sensitivity indices. Finally, conclusions are presented in the last section.

From Morris method to DGSM

Basics of the Morris method

The Morris method is traditionally used as a screening method for problems with a high number of variables for which function evaluations can be CPU-time consuming (see Design of Experiments for Screening). It is composed of individually randomized 'one-factor-at-a-time' (OAT) experiments. Each input factor may assume a discrete number of values, called levels, which are chosen within the factor range of variation.

The sensitivity measures proposed in the original work of Morris [21] are based on what is called an elementary effect. It is defined as follows. The range of each input variable is divided into p levels. Then the elementary effect (incremental ratio) of the i-th input factor is defined as

$$EE_i\left(\mathbf{x}^*\right) = \frac{\left[G\left(x_1^*, \ldots, x_{i-1}^*, x_i^* + \Delta, x_{i+1}^*, \ldots, x_d^*\right) - G\left(\mathbf{x}^*\right)\right]}{\Delta}, \tag{1}$$

where Δ is a predetermined multiple of $1/(p\text{-}1)$ and point $\mathbf{x}^* = \left(x_1^*, \ldots, x_d^*\right) \in H^d$ is such that $x_i^* + \Delta \leq 1$. One can see that the elementary effect are finite difference approximations of the model derivative with respect to x_i and using a large perturbation step Δ.

The distribution of elementary effects EE_i is obtained by randomly sampling R points from H^d. Two sensitivity measures are evaluated for each factor: μ_i an estimate of the mean of the distribution EE_i, and σ_i an estimate of the standard deviation of EE_i. A high value of μ_i indicates an input variable with an important overall influence

on the output. A high value of σ_i indicates a factor involved in interaction with other factors or whose effect is nonlinear. The computational cost of the Morris method is $N_F = R\,(d+1)$.

The revised version of the $EE_i\,(\mathbf{x}^*)$ measure 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 [3]. To avoid the canceling effect which appears in non-monotonic functions Campolongo et al [3] introduced another sensitivity measure μ_i^* based on the absolute value of $EE_i(\mathbf{x}^*)$: $|EE_i(\mathbf{x}^*)|$. It was also noticed that μ_i^* has similarities with the total sensitivity index S_i^{tot} in that it can give a ranking of the variables similar to that based on the S_i^{tot} but no formal proof of the link between μ_i^* and S_i^{tot} was given [3].

Finally, other extensions of the initial Morris method have been introduced for the second-order effects' analysis [2] [4] [6], for the estimation of Morris' measures with any-type of design [26] [32] and for building some 3D Morris' graph [26].

The local sensitivity measure

Consider a differentiable function $G\,(\mathbf{x})$, where $\mathbf{x} = (x_1, \ldots, x_d)$ is a vector of input variables defined in the unit hypercube H^d ($0 \le x_i \le 1$, $i = 1, \ldots, d$). Local sensitivity measures are based on partial derivatives

$$E_i(\mathbf{x}^*) = \frac{\partial G(\mathbf{x}^*)}{\partial x_i}. \tag{2}$$

This measure E_i is the limit version of the elementary effect EE_i defined in (2) when Δ tends to zero. It is its generalization in this sense. In SA, using the partial derivative $\partial G\,/\partial x_i$ is well known as a local method (see Variational Methods). In this paper, the goal is to take advantage of this information in global SA.

The local sensitivity measure $E_i(\mathbf{x}^*)$ depends on a nominal point $\mathbf{x}^*$ and it changes with a change of $\mathbf{x}^*$. This deficiency can be overcome by averaging $E_i(\mathbf{x}^*)$ over

the parameter space H^d. This is done just below, allowing to define new sensitivity measures, called DGSM for Derivative-based Global Sensitivity Measures.

DGSM for uniformly distributed variables

Assume that $\partial G / \partial x_i \in L_2$. Three different DGSM measures are defined:

$$\nu_i = \int_{H^d} \left(\frac{\partial G(\mathbf{x})}{\partial x_i} \right)^2 d\mathbf{x}, \tag{3}$$

$$w_i^{(m)} = \int_{H^d} x_i^m \frac{\partial G(\mathbf{x})}{\partial x_i} d\mathbf{x}, \tag{4}$$

where $m > 0$ is a constant, and

$$\varsigma_i = \frac{1}{2} \int_{H^d} x_i (1 - x_i) \left(\frac{\partial G(\mathbf{x})}{\partial x_i} \right)^2 d\mathbf{x}. \tag{5}$$

DGSM for randomly distributed variables

Consider a function $G(X_1, ..., X_d)$, where $X_1, ..., X_d$ are independent random variables, defined in the Euclidian space R^d, with cumulative density functions (cdfs) $F_1(x_1), ..., F_d(x_d)$. The following DGSM was introduced in Sobol and Kucherenko [38]:

$$\nu_i = \int_{R^d} \left(\frac{\partial G(\mathbf{x})}{\partial x_i} \right)^2 dF(\mathbf{x}) = \mathbb{E} \left[\left(\frac{\partial G(\mathbf{x})}{\partial x_i} \right)^2 \right], \tag{6}$$

with F the joint cdf. A new measure is also introduced:

$$w_i = \int_{R^d} \frac{\partial G(\mathbf{x})}{\partial x_i} dF(\mathbf{x}) = \mathbb{E} \left(\frac{\partial G(\mathbf{x})}{\partial x_i} \right). \tag{7}$$

In (3) and (6), ν_i is in fact the mean value of $(\partial G / \partial x_i)^2$. In the following and in practice, it will be the most useful DGSM.

Sobol' global sensitivity indices

Definitions

The method of global sensitivity indices developed by Sobol' (see Variance-based Sensitivity Analysis: Theory and Estimation Algorithms) is based on ANOVA decom-

position [10]. Consider a square integrable function $G(\mathbf{x})$ defined in the unit hypercube H^d. It can be expanded in the following form

$$G(\mathbf{x}) = g_0 + \sum_i g_i(x_i) + \sum_{i<j} g_{ij}(x_i, x_j) + ... + g_{12...d}(x_1, x_2, ..., x_d). \qquad (8)$$

This decomposition is unique if conditions $\int_0^1 g_{i_1...i_s} dx_{i_k} = 0$ for $1 \leq k \leq s$, are satisfied. Here $1 \leq i_1 < \cdots < i_s \leq d$.

The variances of the terms in the ANOVA decomposition add up to the total variance of the function

$$V = \sum_{s=1}^d \sum_{i_1 < \cdots < i_s}^d V_{i_1...i_s},$$

where $V_{i_1...i_s} = \int_0^1 g_{i_1...i_s}^2(x_{i_1}, ..., x_{i_s}) dx_{i_1}, ..., x_{i_s}$ are called partial variances.

Sobol' defined the global sensitivity indices as the ratios

$$S_{i_1...i_s} = V_{i_1...i_s}/V.$$

All $S_{i_1...i_s}$ are non negative and add up to one:

$$\sum_{i=1}^d S_i + \sum_i \sum_j S_{ij} + \sum_i \sum_j \sum_k S_{ijk}... + S_{1,2,...,d} = 1.$$

Sobol' also defined sensitivity indices for subsets of variables. Consider two complementary subsets of variables y and z:

$$\mathbf{x} = (y, z).$$

Let $y = (x_{i_1}, ..., x_{i_m}), 1 \leq i_1 < ... < i_m \leq d, K = (i_1, ..., i_m)$. The variance corresponding to the set y is defined as

$$V_y = \sum_{s=1}^m \sum_{(i_1 < \cdots < i_s) \in K} V_{i_1...i_s}.$$

V_y includes all partial variances $V_{i_1}, V_{i_2}, ..., V_{i_1...i_s}$ such that their subsets of indices $(i_1, ..., i_s) \in K$.

The total sensitivity indices were introduced by Homma and Saltelli [11]. The total variance V_y^{tot} is defined as

$$V_y^{\text{tot}} = V - V_z.$$

V_y^{tot} consists of all $V_{i_1 \ldots i_s}$ such that at least one index $i_p \in K$ while the remaining indices can belong to the complimentary to K set $\bar{K}$. The corresponding global sensitivity indices are defined as

$$S_y = V_y/V,$$
$$S_y^{\text{tot}} = V_y^{\text{tot}}/V. \tag{9}$$

The important indices in practice are S_i and S_i^{tot}, $i = 1, ..., d$:

$$S_i = V_i/V,$$
$$S_i^{\text{tot}} = V_i^{\text{tot}}/V. \tag{10}$$

Their values in most cases provide sufficient information to determine the sensitivity of the analyzed function to individual input variables. Variance-based methods generally require a large number of function evaluations (see Variance-based Methods: Theory and Algorithms) to achieve reasonable convergence and can become impractical for large engineering problems.

Useful relationships

To present further results on lower and upper bounds of S_i^{tot}, new notations and useful relationships have to be firstly presented. Denote $u_i(\mathbf{x})$ the sum of all terms in the ANOVA decomposition (8) that depend on x_i:

$$u_i(\mathbf{x}) = g_i(x_i) + \sum_{j=1, j \neq i}^{d} g_{ij}(x_i, x_j) + \cdots + g_{12 \ldots d}(x_1, \cdots, x_d). \tag{11}$$

From the definition of ANOVA decomposition it follows that

$$\int_{H^d} u_i(\mathbf{x}) d\mathbf{x} = 0. \tag{12}$$

It is obvious that

$$\frac{\partial G}{\partial x_i} = \frac{\partial u_i}{\partial x_i}.\tag{13}$$

Denote $\mathbf{z} = (x_1, ..., x_{i-1}, x_{i+1}, ..., x_d)$ the vector of all variables but x_i, then $\mathbf{x} \equiv (x_i, \mathbf{z})$ and $G(\mathbf{x}) \equiv G(x_i, \mathbf{z})$. The ANOVA decomposition of $G(\mathbf{x})$ (8) can be presented in the following form

$$G(\mathbf{x}) = u_i(x_i, \mathbf{z}) + v(\mathbf{z}),$$

where $v(\mathbf{z})$ is the sum of terms independent of x_i. Because of (12) it is easy to show that $v(\mathbf{z}) = \int_0^1 G(\mathbf{x})dx_i$. Hence

$$u_i(x_i, \mathbf{z}) = G(\mathbf{x}) - \int_0^1 G(\mathbf{x})dx_i.\tag{14}$$

This equation can be found in Lamboni [18]. The total partial variance V_i^{tot} can be computed as

$$V_i^{\text{tot}} = \int_{H^d} u_i^2(\mathbf{x})d\mathbf{x} = \int_{H^d} u_i^2(x_i, z)dx_i d\mathbf{z}.$$

Then the total sensitivity index S_i^{tot} (10) is equal to

$$S_i^{\text{tot}} = \frac{1}{V} \int_{H^d} u_i^2(\mathbf{x})d\mathbf{x}.\tag{15}$$

A first direct link between total Sobol' sensitivity indices and partial derivatives

Consider continuously differentiable function $G(\mathbf{x})$ defined in the unit hypercube $H^d = [0, 1]^d$. This section presents a theorem that establishes links between the index S_i^{tot} and the limiting values of $|\partial G/\partial x_i|$.

In the case when $\mathbf{y} = (x_i)$, Sobol'-Jansen formula [14][35][31] for D_i^{tot} can be rewritten as

$$D_i^{\text{tot}} = \frac{1}{2} \int_{H^d} \int_0^1 \left[G(\mathbf{x}) - G\left(\overset{\circ}{\mathbf{x}}\right) \right]^2 d\mathbf{x} dx_i',\tag{16}$$

where $\overset{o}{\mathbf{x}} = (x_1, ..., x_{i-1}, x_i', x_{i+1}, ..., x_n)$.

Theorem 1. Assume that $c \le \left|\dfrac{\partial G}{\partial x_i}\right| \le C$, then

$$\frac{c^2}{12V} \le S_i^{\text{tot}} \le \frac{C^2}{12V}. \tag{17}$$

Proof: Consider the increment of $G(\mathbf{x})$ in (16):

$$G(\mathbf{x}) - G\left(\overset{\circ}{\mathbf{x}}\right) = \frac{\partial G(\hat{\mathbf{x}})}{\partial x_i}(x_i - x_i'), \tag{18}$$

where $\hat{\mathbf{x}}$ is a point between $\mathbf{x}$ and $\overset{\circ}{\mathbf{x}}$. Substituting (18) into (16) leads to

$$V_i^{\text{tot}} = \frac{1}{2}\int_{H^d}\int_0^1 \left(\frac{\partial G(\hat{\mathbf{x}})}{\partial x_i}\right)^2 (x_i - x_i')^2 \, d\mathbf{x}dx_i'. \tag{19}$$

In (19) $c^2 \le (\partial G/\partial x_i)^2 \le C^2$ while the remaining integral is

$$\int_0^1 \int_0^1 (x_i' - x_i)^2 \, dx_i' dx_i = \frac{1}{6}.$$

Thus obtained inequalities are equivalent to (17). Consider the function $G = g_0 + c(x_i - 1/2)$. In this case $C = c$, $V = 1/12$ and $S_i^{\text{tot}} = 1$ and the inequalities in (17) become equalities. ∎

DGSM-based bounds for uniformly and normally distributed variables

In this section, several theorems are listed in order to define useful lower and upper bounds of the total Sobol' indices. The proofs of these theorems come from previous works and papers and are not recalled here. Two cases are considered: variables $\mathbf{x}$ following uniform distributions and variables $\mathbf{x}$ following Gaussian distributions. The general case will be seen in a subsequent section.

Uniformly distributed variables

Lower bounds on S_i^{tot}

Theorem 2. There exists the following lower bound between DGSM (3) and the Sobol' total sensitivity index:

$$\frac{\left(\int_{H^d} \left[G\left(1,\mathbf{z}\right) - G\left(0,\mathbf{z}\right)\right] \left[G\left(1,\mathbf{z}\right) + G\left(0,\mathbf{z}\right) - 2G\left(\mathbf{x}\right)\right] d\mathbf{x}\right)^2}{4\nu_i V} < S_i^{\text{tot}} \qquad (20)$$

Proof: The proof of this Theorem is given in Kucherenko and Song [16] and is based on equation (15) and a Cauchy-Schwartz inequality applied on $\int_{H^d} u_i(\mathbf{x})\frac{\partial u_i(\mathbf{x})}{\partial x_i} d\mathbf{x}$. ∎

The lower bound number number one (LB1) is defined as

$$\frac{\left(\int_{H^d} \left[G\left(1,\mathbf{z}\right) - G\left(0,\mathbf{z}\right)\right] \left[G\left(1,\mathbf{z}\right) + G\left(0,\mathbf{z}\right) - 2G\left(\mathbf{x}\right)\right] d\mathbf{x}\right)^2}{4\nu_i V}.$$

Theorem 3. There exists the following lower bound, denoted $\gamma(m)$, between DGSM (4) and the Sobol' total sensitivity index:

$$\gamma(m) = \frac{(2m+1)\left[\int_{H^d}\left(G(1,\mathbf{z}) - G(\mathbf{x})\right) d\mathbf{x} - w_i^{(m+1)}\right]^2}{(m+1)^2 V} < S_i^{\text{tot}}. \qquad (21)$$

Proof: The proof of this Theorem in given in Kucherenko and Song [16] and is based on equation (15) and a Cauchy-Schwartz inequality applied on $\int_{H^d} x_i^m u_i(\mathbf{x}) d\mathbf{x}$. ∎

In fact, Theorem 3 gives a set of lower bounds depending on parameter m. The value of m at which $\gamma(m)$ attains its maximum is of particular interest. Further, star (*) is used to denote such a value m: $m^* = \arg\max(\gamma(m))$. $\gamma(m^*)$ is called the lower bound number two (LB2):

$$\gamma(m^*) = \frac{(2m^* + 1)\left[\int_{H^d}\left(G(1,\mathbf{z}) - G(\mathbf{x})\right) d\mathbf{x} - w_i^{(m^*+1)}\right]^2}{(m^* + 1)^2 V} \qquad (22)$$

The maximum lower bound LB* is defined as

$$\text{LB*} = \max(\text{LB1},\text{LB2}). \qquad (23)$$

Both lower and upper bounds can be estimated by a set of derivative based measures:

$$\Upsilon_i = \{\nu_i, w_i^{(m)}, \zeta_i\}, \ m > 0. \qquad (24)$$

Upper bounds on S_i^{tot}

Theorem 4. There exists the following upper bound between DGSM (3) and the Sobol' total sensitivity index:

$$S_i^{\text{tot}} \leq \frac{\nu_i}{\pi^2 V}. \tag{25}$$

Proof: The proof of this Theorem in given in Sobol and Kucherenko [38]. It is based on inequality:

$$\int_0^1 u^2(x)\, dx \leq \frac{1}{\pi^2} \int_0^1 \left(\frac{\partial u}{\partial x}\right)^2 dx$$

and relationships (13) and (15). ∎

Consider the set of values $\nu_1, ..., \nu_d$, $1 \leq i \leq d$. One can expect that smaller ν_i correspond to less influential variables x_i. This importance criterion is similar to the modified Morris importance measure μ^*, whose limiting values are

$$\mu_i^* = \int_{H^d} \left|\frac{\partial G(\mathbf{x})}{\partial x_i}\right| d\mathbf{x}.$$

From a practical point of view the criteria μ_i and ν_i are equivalent: they are evaluated by the same numerical algorithm and are linked by relations $\nu_i \leq C\mu_i$ and $\mu_i \leq \sqrt{\nu_i}$.

The right term in (25) is further called the upper bound number one (UB1).

Theorem 5. There exists the following upper bound between DGSM (5) and the Sobol' total sensitivity index:

$$S_i^{\text{tot}} \leq \frac{\varsigma_i}{V}. \tag{26}$$

Proof: The following inequality [10] is used:

$$0 \leq \int_0^1 u^2 dx - \left(\int_0^1 u\, dx\right)^2 \leq \frac{1}{2}\int_0^1 x(1-x)u'^2 dx. \tag{27}$$

The inequality is reduced to an equality only if u is constant. Assume that u is given by (11), then $\int_0^1 u\, dx = 0$. From (27), equation (26) is obtained. ∎

Further ς_i/D is called the upper bound number two (UB2). Note that $\frac{1}{2}x_i(1-x_i)$

for $0 \le x_i \le 1$ is bounded: $0 \le \frac{1}{2}x_i(1 - x_i) \le 1/8$. Therefore, $0 \le \varsigma_i \le \nu_i/8$.

Normally distributed variables

Lower bound on S_i^{tot}

Theorem 6. If X_i is normally distributed with a mean μ_i and a finite variance σ_i^2, there

exists the following lower bound between DGSM (7) and the Sobol' total sensitivity

index:

$$\frac{\sigma_i^4}{(\mu_i^2 + \sigma_i^2)V}w_i^2 \le S_i^{\text{tot}}. \tag{28}$$

Proof: Using the equation (15) and Cauchy-Schwartz inequality applied on $\int_{R^d} x_i u_i(\mathbf{x})dF(\mathbf{x})$

(with F the joint cdf), Kucherenko and Song [16] give the proof of this inequality when

$\mu_i = 0$ (omitting to mention this condition). The general proof, obtained by Petit [25],

is given below.

Consider a univariate function $g(X)$, with X a normally distributed variable

with mean μ, finite variance σ^2 and cdf F. With adequate conditions on g, the following

equality is obtained by integrating by parts:

$$\mathbb{E}[g'(X)] = \int_{-\infty}^{\infty} g'(x)dF(x) = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} g'(x)\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]dx$$

$$= \frac{1}{\sigma\sqrt{2\pi}}\left[g(x)\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]\right]_{-\infty}^{+\infty} + \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} g(x)\frac{x-\mu}{\sigma^2}\exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]dx$$

$$= \frac{1}{\sigma^2} \int_{-\infty}^{\infty} xg(x)dF(x) - \mu \int_{-\infty}^{\infty} g(x)dF(x).$$

In this equation, replacing $g(x)$ by $u_i(\mathbf{x})$ with x_i normally distributed, the w_i

DGSM writes

$$w_i = \int_{R^d} \frac{\partial G(\mathbf{x})}{\partial x_i}dF(\mathbf{x}) = \int_{R^d} \frac{\partial u_i(\mathbf{x})}{\partial x_i}dF(\mathbf{x}) = \frac{1}{\sigma_i^2} \int_{R^d} x_i u_i(\mathbf{x})dF(\mathbf{x}),$$

because $\int_{R^d} u_i(\mathbf{x})dF(\mathbf{x}) = 0$ (due to the ANOVA decomposition condition). Moreover,

the Cauchy-Schwartz inequality applied on $\int_{R^d} x_i u_i(\mathbf{x})dF(\mathbf{x})$ gives

$$\left[\int_{R^d} x_i u_i(\mathbf{x}) dF(\mathbf{x})\right]^2 \leq \int_{R^d} x_i^2 dF(\mathbf{x}) \int_{R^d} [u_i(\mathbf{x})]^2 dF(\mathbf{x}).$$

Combining the two latter equations leads to the expression

$$w_i^2 \leq \frac{1}{\sigma_i^4}(\mu_i^2 + \sigma_i^2) V S_i^{\text{tot}},$$

which is equivalent to Eq. (28). ∎

Upper bounds on S_i^{tot}

The following Theorem 7 is a generalization of Theorem 1.

Theorem 7. If X_i has a finite variance σ_i^2 and $c \leq \left|\dfrac{\partial G}{\partial x_i}\right| \leq C$, then

$$\frac{\sigma_i^2 c^2}{V} \leq S_i^{\text{tot}} \leq \frac{\sigma_i^2 C^2}{V}. \tag{29}$$

The constant factor σ_i^2 cannot be improved.

Theorem 8. If X_i is normally distributed with a finite variance σ_i^2, there exists the following upper bound between DGSM (6) and the Sobol' total sensitivity index:

$$S_i^{\text{tot}} \leq \frac{\sigma_i^2}{V}\nu_i. \tag{30}$$

The constant factor σ_i^2 cannot be reduced.

Proof: The proofs of these Theorems are presented in Sobol and Kucherenko [38]. ∎

DGSM-based bounds for groups of variables

Let $\mathbf{x} = (x_1, ..., x_d)$ be a point in the $d-$dimensional unit hypercube with Lebesgue measure $d\mathbf{x} = dx_1 \cdots dx_d$. Consider an arbitrary subset of the variables $y = (x_{i_1}, ..., x_{i_s})$, $1 \leq i_1 \leq ... \leq i_s \leq d$, and the set of remaining complementary variables z, so that $\mathbf{x} = (y, z)$, $d\mathbf{x} = dy\, dz$. Further all the integrals are written without integration limits, by assuming that each integration variable varies independently from 0 to 1.

Consider the following DGSM τ_y:

$$\tau_y = \sum_{p=1}^s \int \left(\frac{\partial G\left(\mathbf{x}\right)}{\partial x_{i_p}} \right)^2 \frac{1 - 3x_{i_p} + 3x_{i_p}^2}{6} d\mathbf{x}. \tag{31}$$

Theorem 9. If $G\left(\mathbf{x}\right)$ is linear with respect to $x_{i_1}, ..., x_{i_s}$, then $V_y^{\text{tot}} = \tau_y$, or in other words $S_y^{\text{tot}} = \frac{\tau_y}{V}$.

Theorem 10. The following general inequality holds: $V_y^{\text{tot}} \leq \left(24/\pi^2\right)\tau_y$, or in other words $S_y^{\text{tot}} \leq \frac{24}{\pi^2 V}\tau_y$.

Proof: The proofs of these Theorems are given in Sobol and Kucherenko [39]. The second theorem shows that small values of τ_y imply small values of S_y^{tot} and this allows identification of a set of unessential factors y (usually defined by a condition of the type $S_y^{\text{tot}} < \epsilon$, where ϵ is small). ∎

Importance criterion τ_i

Consider the one dimensional case when the subset y consists of only one variable $y = (x_i)$, then measure $\tau_y = \tau_i$ has the form

$$\tau_i = \int \left(\frac{\partial G\left(\mathbf{x}\right)}{\partial x_i} \right)^2 \frac{1 - 3x_i + 3x_i^2}{6} d\mathbf{x}. \tag{32}$$

It is easy to show that $\nu_i/24 \leq \tau_i \leq \nu_i/6$. From UB1 it follows that

$$S_i^{\text{tot}} \leq \frac{24}{\pi^2 V}\tau_i. \tag{33}$$

Thus small values of τ_i imply small values of S_i^{tot}, that are characteristic for non important variables x_i. At the same time, the following corollary is obtained from Theorem 9: if $G\left(\mathbf{x}\right)$ depends linearly on x_i, then $S_i^{\text{tot}} = \tau_i/V$. Thus τ_i is closer to V_i^{tot} than ν_i.

Note that the constant factor $1/\pi^2$ in (25) is the best possible. But in the general inequality for τ_i (33) the best possible constant factor is unknown.

There is a general link between importance measures τ_i, ς_i and ν_i:

$$\tau_i = -\varsigma_i + \frac{1}{6}\nu_i,$$

then

$$\varsigma_i = \frac{1}{6}\nu_i - \tau_i.$$

Normally distributed random variables

Consider independent normal random variables $X_1, ..., X_d$ with parameters $(\mu_i, \sigma_i)_{i=1...d}$.

Define τ_i as

$$\tau_i = \frac{1}{2}\mathbb{E}\left[\left(\frac{\partial G(\mathbf{x})}{\partial x_i}\right)^2 (x_i' - x_i)^2\right].$$

The expectation over x_i' can be computed analytically. Then

$$\tau_i = \frac{1}{2}\mathbb{E}\left[\left(\frac{\partial G(\mathbf{x})}{\partial x_i}\right)^2 \frac{(x_i - \mu_i)^2 + \sigma_i^2}{2}\right].$$

Theorem 11. If $X_1, ..., X_d$ are independent normal random variables, then for an arbitrary subset y of these variables, the following inequality is obtained:

$$S_y^{\text{tot}} \leq \frac{2}{V}\tau_y.$$

Proof: The proof is given in Sobol and Kucherenko [39]. ∎

DGSM-based upper bounds in the general case

As previously, consider the function $G(X_1, ..., X_d)$, where $X_1, ..., X_d$ are independent random variables, defined in the Euclidian space R^d, with cdfs $F_1(x_1), ..., F_d(x_d)$. Assume further that each X_i admits a probability density function (pdf), denoted by $f_i(x_i)$. In the following, all the integrals are written without integration limits.

The developments in this section are based on the classical L^2-Poincaré inequality:

$$\int G(\mathbf{x})^2 dF(\mathbf{x}) \leq C(F) \int \|\nabla G(\mathbf{x})\|^2 dF(\mathbf{x}) \tag{34}$$

where F is the joint cdf of $(X_1, ..., X_d)$. (34) is valid for all functions G in $L^2(F)$ such that $\int G(\mathbf{x})dF(\mathbf{x}) = 0$ and $\|\nabla f\| \in L^2(F)$. The constant $C(F)$ in Eq. (34) is called a Poincaré constant of F. In some cases, it exists and optimal Poincaré constant $C_{\text{opt}}(F)$ which is the best possible constant. In measure theory, the Poincaré constants are expressed as a function of so-called Cheeger constants [1] which are used for SA in Lamboni et al [19] (see Roustant et al [28] for more details).

A connection between total indices and DGSM has been established by Lamboni et al [19] for variables with continuous distributions (called Boltzmann probability measures in their paper).

Theorem 12. Let F_i and f_i be respectively the cdf and the pdf of X_i, the following inequality is obtained:

$$S_i^{\text{tot}} \leq \frac{C(F_i)}{V}\nu_i,$$ (35)

with ν_i the DGSM defined in Eq. (6) and

$$C(F_i) = 4\left[\sup_{x \in \mathbb{R}}\frac{\min\left(F_i(x), 1 - F_i(x)\right)}{f_i(x)}\right]^2.$$ (36)

Proof: This result comes from the direct application of the L^2-Poincaré inequality (34) on $u_i(\mathbf{x})$ (see Eq. (11)). ∎

In Lamboni et al [19] and Roustant et al [28], the particular case of log-concave probability distribution has been developed. It includes classical distributions as for instance the normal, exponential, Beta, Gamma and Gumbel distributions. In this case, the constant writes

$$C(F_i) = \frac{1}{f_i(\tilde{m}_i)^2}$$ (37)

with $\tilde{m}_i$ the median of the distribution F_i. This allows to obtain analytical expressions for $C(F_i)$ in several cases [19]. In the case of a log-concave truncated distribution on $[a, b]$, the constant writes [28]

$$(F_i(b) - F_i(a))^2 / f_i\left(q_i\left(\frac{F_i(a) + F_i(b)}{2}\right)\right)^2$$ (38)

with $q_i(\cdot)$ the quantile function of X_i. Table 1 gives some examples of Poincaré constants for several well-known and often used probability distributions in practice.

Distribution	Poincaré constant	Optimal constant
Uniform $\mathcal{U}[a\,b]$	$(b-a)^2/\pi^2$	yes
Normal $\mathcal{N}(\mu,\sigma^2)$	σ^2	yes
Exponential $\mathcal{E}(\lambda)$, $\lambda > 0$	$\dfrac{4}{\lambda^2}$	yes
Gumbel $\mathcal{G}(\mu,\beta)$, scale $\beta > 0$	$\left(\dfrac{2\beta}{\log 2}\right)^2$	no
Weibull $\mathcal{W}(k,\lambda)$, shape $k \geq 1$, scale $\lambda > 0$	$\left[\dfrac{2\lambda(\log 2)^{(1-k)/k}}{k}\right]^2$	no

Table 1. Poincaré constants for a few probability distributions.

For studying second-order interactions, Roustant et al [28] have derived a similar to (35) inequality based on the squared crossed derivatives of the function. Assuming that second-order derivatives of G are in $L^2(F)$, it uses the so-called crossed-DGSM

$$\nu_{ij} = \int \left(\frac{\partial^2 G(\mathbf{x})}{\partial x_i \partial x_j}\right)^2 dF(\mathbf{x}), \tag{39}$$

introduced by Friedman and Popescu [7]. An inequality link is made with an extension of the total Sobol' sensitivity indices to general sets of variables (called superset importance or total interaction index) proposed by Liu and Owen [20]. In the case of a pair of variables $\{X_i, X_j\}$, the superset importance is defined as

$$V_{ij}^{\text{super}} = \sum_{I \supseteq \{i,j\}} V_I. \tag{40}$$

The estimation methods of this total interaction index have also been studied by Fruth et al [8].

Theorem 13. For all pairs $\{i,j\}$ ($1 \leq i < j \leq d$),

$$V_{ij} \leq V_{ij}^{\text{super}} \leq C(F_i)C(F_j)\nu_{ij}. \tag{41}$$

These inequalities with the corresponding Sobol' indices write

$$S_{ij} \leq S_{ij}^{\text{super}} \leq \frac{C(F_i)C(F_j)}{V}\nu_{ij}. \tag{42}$$

Roustant et al [28] have shown on several examples how to apply this result in order to detect pairs of inputs that do not interact together (see also Muehlenstaedt et al [22] and Fruth et al [8] which use Sobol' indices).

Computational costs

All DGSM can be computed using the same set of partial derivatives $\frac{\partial G(\mathbf{x})}{\partial x_i}$, $i = 1,...,d$. Evaluation of $\frac{\partial G(\mathbf{x})}{\partial x_i}$ can be done analytically for explicitly given easily-differentiable functions or numerically:

$$\frac{\partial G(\mathbf{x}^*)}{\partial x_i} = \frac{\left[G\left(x_1^*,\ldots,x_{i-1}^*,x_i^*+\delta,x_{i+1}^*,\ldots,x_n^*\right) - G\left(\mathbf{x}^*\right)\right]}{\delta}. \tag{43}$$

This is called a finite-difference scheme (see Variational Methods) with δ which is a small increment. There is a similarity with the elementary effect formula (2) of the Morris method which is however computed with large Δ.

In the case of straightforward numerical estimations of all partial derivatives (43) and computation of integrals using MC or QMC methods, the number of required function evaluations for a set of all input variables is equal to $N(d+1)$, where N is a number of sampled points. Computing LB1 also requires values of $G\left(0, \mathbf{z}\right), G\left(1, \mathbf{z}\right)$, while computing LB2 requires only values of $G\left(1, \mathbf{z}\right)$. In total, numerical computation of LB* for all input variables would require $N_G^{\text{LB}*} = N(d+1) + 2Nd = N(3d+1)$ function evaluations. Computation of all upper bounds require $N_G^{\text{UB}} = N(d+1)$ function evaluations. This is the same number that the number of function evaluations required for computation of S_i^{tot} which is $N_G^S = N(d+1)$ [31].

However, the number of sampled points N needed to achieve numerical convergence can be different for DGSM and S_i^{tot}. It is generally lower for the case of

DGSM. Moreover, the numerical efficiency of the DGSM method can be significantly increased by using algorithmic differentiation in the adjoint (reverse) mode [9] (see also Variational Methods). This approach allows estimating all derivatives at a cost independent of d, at most 4-6 times of that for evaluating the original function $G(\mathbf{x})$ [13].

Test cases

In this section, three test cases are considered, in order to illustrate application of DGSM and their links with S_i^{tot}.

Example 1. Consider a linear with respect to x_i function:

$$G(x) = a(\mathbf{z})x_i + b(\mathbf{z}).$$

For this function $S_i = S_i^{\text{tot}}$, $V_i^{\text{tot}} = \dfrac{1}{12}\displaystyle\int_{H^{d-1}} a^2(\mathbf{z})d\mathbf{z}$, $\nu_i = \displaystyle\int_{H^{d-1}} a^2(\mathbf{z})d\mathbf{z}$, LB1 $= \dfrac{\left(\int_{H^d}\left(a^2(\mathbf{z})-2a^2(\mathbf{z})x_i\right)d\mathbf{z}dx_i\right)^2}{4V\int_{H^{d-1}} a^2(\mathbf{z})d\mathbf{z}} = 0$ and $\gamma(m) = \dfrac{(2m+1)m^2\left(\int_{H^{d-1}} a(\mathbf{z})d\mathbf{z}\right)^2}{4(m+2)^2(m+1)^2 V}$. A maximum value of $\gamma(m)$ is attained at m^*=3.745, while $\gamma^*(m^*) = \dfrac{0.0401}{V}\left(\displaystyle\int a(\mathbf{z})d\mathbf{z}\right)^2$. The lower and upper bounds are LB* $\approx 0.48 S_i^{\text{tot}}$, UB1 $\approx 1.22 S_i^{\text{tot}}$. UB2 $= \dfrac{1}{12V}\displaystyle\int_0^1 a(\mathbf{z})^2 d\mathbf{z} = S_i^{\text{tot}}$.

For this test function UB2 < UB1.

Example 2. Consider the so-called g-function which is often used in global SA for illustration purposes:

$$G(x) = \prod_{i=1}^d v_i,$$

where $v_i = \dfrac{|4x_i - 2| + a_i}{1 + a_i}$, $a_i (i = 1, ..., d)$ are constants. It is easy to see that for this function $g_i(x_i) = (v_i - 1)$, $u_i(x) = (v_i - 1)\prod_{j=1, j\neq i}^d v_j$ and as a result LB1=0. The total variance is $V = -1 + \prod_{j=1}^d \left(1 + \dfrac{1/3}{(1+a_j)^2}\right)$. The analytical values of S_i, S_i^{tot} and LB2 are given in Table 2.

Table 2. The analytical expressions for S_i, S_i^{tot} and LB2 for g-function.

S_i	S_i^{tot}	$\gamma(m)$
$\dfrac{1/3}{(1+a_i)^2 V}$	$\dfrac{\frac{1/3}{(1+a_i)^2}\prod_{j=1,j\neq i}^d \left(1+\frac{1/3}{(1+a_j)^2}\right)}{V}$	$\dfrac{(2m+1)\left[1-\frac{4\left(1-(1/2)^{m+1}\right)}{m+2}\right]^2}{(1+a_i)^2(m+1)^2 V}$

By solving equation $\dfrac{d\gamma(m)}{dm} = 0$, m^*=9.64 and $\gamma(m^*) = \dfrac{0.0772}{(1+a_i)^2 V}$. It is interesting to note that m^* does not depend on a_i, $i = 1, 2, ..., d$ and d. In the extreme cases: if $a_i \to \infty$ for all i, $\dfrac{\gamma(m^*)}{S_i^{\text{tot}}} \to 0.257$, $\dfrac{S_i}{S_i^{\text{tot}}} \to 1$, while if $a_i \to 0$ for all i, $\dfrac{\gamma(m^*)}{S_i^{\text{tot}}} \to \dfrac{0.257}{(4/3)^{d-1}}$, $\dfrac{S_i}{S_i^{\text{tot}}} \to \dfrac{1}{(4/3)^{d-1}}$. The analytical expression for S_i^{tot}, UB1 and UB2 are given in Table 3.

Table 3. The analytical expressions for S_i^{tot}, UB1 and UB2 for g-function.

S_i^{tot}	UB1	UB2
$\dfrac{\frac{1/3}{(1+a_i)^2}\prod_{j=1,j\neq i}^d \left(1+\frac{1/3}{(1+a_j)^2}\right)}{V}$	$\dfrac{16\prod_{j=1,j\neq i}^d \left(1+\frac{1/3}{(1+a_j)^2}\right)}{(1+a_i)^2\pi^2 V}$	$\dfrac{4\prod_{j=1,j\neq i}^d \left(1+\frac{1/3}{(1+a_j)^2}\right)}{3(1+a_i)^2 V}$

For this test function $\dfrac{S_i^{\text{tot}}}{\text{UB1}} = \dfrac{\pi^2}{48}$, $\dfrac{S_i^{\text{tot}}}{\text{UB2}} = \dfrac{1}{4}$, hence $\dfrac{\text{UB2}}{\text{UB1}} = \dfrac{\pi^2}{12} < 1$.

Values of S_i, S_i^{tot}, UB1, UB2 and LB2 for the case of $\boldsymbol{a}$=[0,1,4.5,9,99,99,99,99], d=8 are given in Table 4 and shown in Fig. 1. One can see that the knowledge of LB2 and UB1 allows to rank correctly all the variables in the order of their importance.

Table 4. Values of LB*, S_i, S_i^{tot}, UB1 and UB1. Example 2, $\boldsymbol{a}$=[0,1,4.5,9,99,99,99,99], d=8.

	x_1	x_2	x_3	x_4	$x_5...x_8$
LB*	0.166	0.0416	0.00549	0.00166	0.000017
S_i	0.716	0.179	0.0237	0.00720	0.0000716
S_i^{tot}	0.788	0.242	0.0343	0.0105	0.000105
UB1	3.828	1.178	0.167	0.0509	0.00051
UB2	3.149	0.969	0.137	0.0418	0.00042

Example 3. Consider the reduced Morris' test function with four inputs [3]:
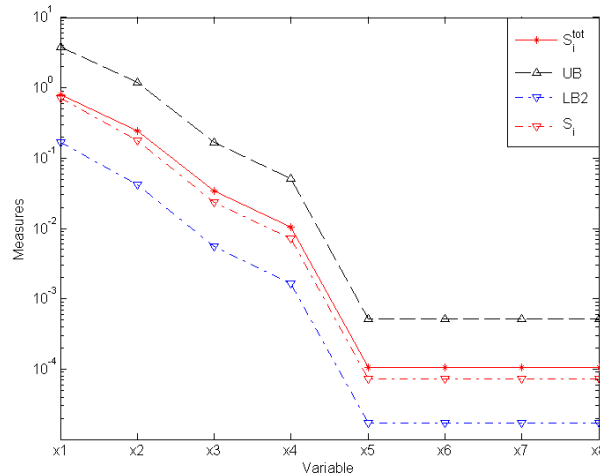
Fig. 1. Values of S_i, S_i^{tot}, LB2 and UB1 for all input variables. Example 2 with $\mathbf{a} = [0, 1, 4.5, 9, 99, 99, 99, 99]$, $d = 8$.

$$f(\boldsymbol{x}) = \sum_{i=1}^{4} b_i x_i + \sum_{i \leq j}^{4} b_{ij} x_i x_j + \sum_{i \leq j \leq k}^{4} b_{ijk} x_i x_j x_k \tag{44}$$

with $b_i = \begin{bmatrix} 0.05 \\ 0.59 \\ 10 \\ 0.21 \end{bmatrix}$, $b_{ij} = \begin{bmatrix} 0 & 80 & 60 & 40 \\ 0 & 30 & 0.73 & 0.18 \\ 0 & 0 & 0.64 & 0.93 \\ 0 & 0 & 0 & 0.06 \end{bmatrix}$, $b_{ij4} = \begin{bmatrix} 0 & 10 & 0.98 & 0.19 \\ 0 & 0 & 0.49 & 50 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$.

The indices $b_{ijk} \; \forall \; k \neq 4$ are null.

The four input variables x_i $(i = 1, \ldots, 4)$ follow uniform distribution on $[0, 1]$. Sobol' indices are computed via the Monte-carlo scheme of Saltelli [29] (using two initial matrices of size 10^5), while DGSM are computed with Monte-Carlo sampling of size n (using derivatives computing by finite differences (43) with $\delta = 10^{-5}$), with n ranging from 20 to 500, Figure 2 shows that DGSM bounds UB1$_i$ are greater than the total Sobol' indices S_{T_i} (for $i = 1, 2, 3, 4$) as expected, except for $n < 30$ which is a too small sample size. For small S_{T_i}, UB1$_i$ is close to the S_{T_i} value. It confirms that DGSM bounds are first useful for screening exercises. Other numerical tests involving non-uniform and non-normal distributions for the inputs can be found in Lamboni et al [19] and Fruth et al [8].
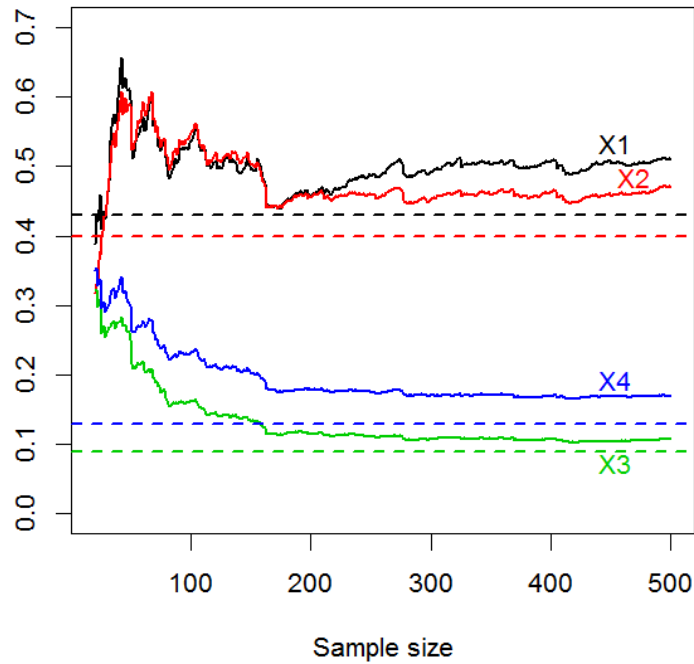
Fig. 2. For the 4 input variables of the reduced Morris' test function: Convergence of the DGSM bound estimates (solid lines) in function of the sample size and comparison to theoretical values of total Sobol' indices S_{T_i} (dashed lines).

Conclusions

This paper has shown that using lower and upper bounds based on DGSM is possible in most cases to get a good practical estimation of the values of S_i^{tot} at a fraction of the CPU cost for estimating S_i^{tot}. Upper and lower bounds can be estimated using MC/QMC integration methods using the same set of partial derivative values. Most of the applications show that DGSM can be used for fixing unimportant variables and subsequent model reduction because small values of DGSM imply small values of S_i^{tot}. In a general case variable ranking can be different for DGSM and variance based methods but for linear function and product function, DGSM can give the same variable ranking as S_i^{tot}.

Engineering applications of DGSM can be found for instance in Kiparissides et al [15] and Rodriguez-Fernandez et al [27] for biological systems modeling, Patelli et al [24] for structural mechanics, Iooss et al [12] for an aquatic prey-predator model, Petit [25] for a river flood model and Touzany and Busby [41] for an hydrogeological simulator of the oil industry. One of the main prospect in practical situations is to use algorithmic differentiation in the reverse (adjoint) mode on the numerical model, allowing to estimate efficiency all partial derivatives of this model (see Variational Methods). In this case, the cost of DGSM estimations would be independent of the number of input variables. Obtaining global sensitivity information in a reasonable cpu time cost is therefore possible even for large-dimensional model (several tens and spatially distributed inputs in the recent and pioneering attempt of Petit [25]). When the adjoint model is not available, the DGSM estimation remains a problem in high dimension and novel ideas have to be explored [23] [24]. Coupling DGSM with non-parametric regression techniques or metamodel-based technique (see Metamodel-based sensitivity analysis: Polynomial chaos expansions and Gaussian processes) is another research prospect as first shown by Sudret and Mai [40] and De Lozzo and Marrel [5].

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