

Derivative-based Global Sensitivity Measures and Their Link with Sobol' Sensitivity Indices

Sergei Kucherenko and Shufang Song

Abstract The variance-based method of Sobol' sensitivity indices is very popular among practitioners due to its efficiency and easiness of interpretation. However, for high-dimensional models the direct application of this method can be very time-consuming and prohibitively expensive to use. One of the alternative global sensitivity analysis methods known as the method of derivative based global sensitivity measures (DGSM) has recently become popular among practitioners. It has a link with the Morris screening method and Sobol' sensitivity indices. 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. We present a survey of recent advances in DGSM and new results concerning new 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: Global sensitivity analysis; Monte Carlo methods; Quasi Monte Carlo methods; Derivative based global measures; Morris method; Sobol sensitivity indices

1 Introduction

Global sensitivity analysis (GSA) is the study of how the uncertainty in the model output is apportioned to the uncertainty in model inputs [9],[14]. GSA can provide valuable information regarding the dependence of the model output to its input parameters. The variance-based method of global sensitivity indices developed by Sobol' [11] became very popular among practitioners due to its efficiency and eas-

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iness of interpretation. 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 [3]. The total sensitivity indices are used to identify non-important variables which can then be fixed at their nominal values to reduce model complexity [9]. For high-dimensional models the direct application of variance-based GSA measures can be extremely time-consuming and impractical.

A number of alternative SA techniques have been proposed. In this paper we present 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. These measures were briefly introduced by Sobol' and Gershman in [12]. Kucherenko *et al* [6] introduced some other derivative-based global sensitivity measures (DGSM) and coined the acronym DGSM. They showed that the computational cost of numerical evaluation of DGSM can be much lower than that for estimation of Sobol' sensitivity indices which later was confirmed in other works [5]. DGSM can be seen as a generalization and formalization of the Morris importance measure also known as elementary effects [8]. Sobol' and Kucherenko[15] proved theoretically that 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} . They also introduced modified DGSM which can be used for both a single input and groups of inputs [16]. Such measures can be applied for problems with a high number of input variables to reduce the computational time. Lamboni *et al* [7] extended results of Sobol' and Kucherenko for models with input variables belonging to the class of Boltzmann probability measures.

The numerical efficiency of the DGSM method can be improved by using the automatic differentiation algorithm for calculation DGSM as was shown in [5]. 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 [1]. It allows estimating all derivatives at a cost at most 4-6 times of that for evaluating the original function [4].

This paper is organised as follows: Section 2 presents Sobol' global sensitivity indices. DGSM and lower and upper bounds on total Sobol' sensitivity indices for uniformly distributed variables and random variables are presented in Sections 3 and 4, respectively. In Section 5 we consider test cases which illustrate an application of DGSM and their links with total Sobol' sensitivity indices. Finally, conclusions are presented in Section 6.

2 Sobol' global sensitivity indices

The method of global sensitivity indices developed by Sobol' is based on ANOVA decomposition [11]. Consider the square integrable function $f(\mathbf{x})$ defined in the unit hypercube $H^d = [0, 1]^d$. The decomposition of $f(\mathbf{x})$

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^d f_i(x_i) + \sum_{i=1}^d \sum_{j>i} f_{ij}(x_i, x_j) + \cdots + f_{12\dots d}(x_1, \dots, x_d), \quad (1)$$

where $f_0 = \int_{H^d} f(\mathbf{x}) d\mathbf{x}$, is called ANOVA if conditions

$$\int_{H^d} f_{i_1\dots i_s} dx_{i_k} = 0 \quad (2)$$

are satisfied for all different groups of indices x_1, \dots, x_s such that $1 \leq i_1 < i_2 < \dots < i_s \leq d$. These conditions guarantee that all terms in (1) are mutually orthogonal with respect to integration.

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

$$D = \int_{H^d} f^2(\mathbf{x}) d\mathbf{x} - f_0^2 = \sum_{s=1}^d \sum_{i_1 < \dots < i_s} D_{i_1\dots i_s},$$

where $D_{i_1\dots i_s} = \int_{H^d} f_{i_1\dots i_s}^2(x_{i_1}, \dots, x_{i_s}) dx_{i_1}, \dots, x_{i_s}$ are called partial variances.

Total partial variances account for the total influence of the factor x_i :

$$D_i^{tot} = \sum_{\langle i \rangle} D_{i_1\dots i_s},$$

where the sum $\sum_{\langle i \rangle}$ is extended over all different groups of indices x_1, \dots, x_s satisfying condition $1 \leq i_1 < i_2 < \dots < i_s \leq n$, $1 \leq s \leq n$, where one of the indices is equal to i . The corresponding total sensitivity index is defined as

$$S_i^{tot} = D_i^{tot} / D.$$

Denote $u_i(\mathbf{x})$ the sum of all terms in ANOVA decomposition (1) that depend on x_i :

$$u_i(\mathbf{x}) = f_i(x_i) + \sum_{j=1, j \neq i}^d f_{ij}(x_i, x_j) + \cdots + f_{12\dots d}(x_1, \dots, x_d).$$

From the definition of ANOVA decomposition it follows that

$$\int_{H^d} u_i(\mathbf{x}) d\mathbf{x} = 0. \quad (3)$$

The total partial variance D_i^{tot} can be computed as

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

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

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

where $v(\mathbf{z})$ is the sum of terms independent of x_i . Because of (2) and (3) it is easy to show that $v(\mathbf{z}) = \int_{H^d} f(\mathbf{x}) dx_i$. Hence

$$u_i(x_i, \mathbf{z}) = f(\mathbf{x}) - \int_{H^d} f(\mathbf{x}) dx_i. \quad (4)$$

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

$$S_i^{tot} = \frac{\int_{H^d} u_i^2(\mathbf{x}) d\mathbf{x}}{D}. \quad (5)$$

We note that in the case of independent random variables all definitions of the ANOVA decomposition remain to be correct but all derivations should be considered in probabilistic sense as shown in [14] and presented in Section 4.

3 DGSM for uniformly distributed variables

Consider continuously differentiable function $f(\mathbf{x})$ defined in the unit hypercube $H^d = [0, 1]^d$ such that $\partial f / \partial x_i \in L_2$.

Theorem 1. Assume that $c \leq \left| \frac{\partial f}{\partial x_i} \right| \leq C$. Then

$$\frac{c^2}{12D} \leq S_i^{tot} \leq \frac{C^2}{12D}. \quad (6)$$

The proof is presented in [15].

The Morris importance measure also known as elementary effects originally defined as finite differences averaged over a finite set of random points [8] was generalized in [6]:

$$\mu_i = \int_{H^d} \left| \frac{\partial f(\mathbf{x})}{\partial x_i} \right| d\mathbf{x}. \quad (7)$$

Kucherenko *et al* [6] also introduced a new DGSM measure:

$$v_i = \int_{H^d} \left(\frac{\partial f(\mathbf{x})}{\partial x_i} \right)^2 d\mathbf{x}. \quad (8)$$

In this paper we define two new DGSM measures:

$$w_i^{(m)} = \int_{H^d} x_i^m \frac{\partial f(\mathbf{x})}{\partial x_i} d\mathbf{x}, \quad (9)$$

where m is a constant, $m > 0$,

$$\varsigma_i = \frac{1}{2} \int_{H^d} x_i(1-x_i) \left(\frac{\partial f(\mathbf{x})}{\partial x_i} \right)^2 d\mathbf{x}. \quad (10)$$

We note that v_i is in fact the mean value of $(\partial f / \partial x_i)^2$. We also note that

$$\frac{\partial f}{\partial x_i} = \frac{\partial u_i}{\partial x_i}. \quad (11)$$

3.1 Lower bounds on S_i^{tot}

Theorem 2. There exists the following lower bound between DGSM (8) and the Sobol' total sensitivity index

$$\frac{\left(\int_{H^d} [f(1, \mathbf{z}) - f(0, \mathbf{z})] [f(1, \mathbf{z}) + f(0, \mathbf{z}) - 2f(\mathbf{x})] d\mathbf{x} \right)^2}{4v_i D} < S_i^{tot}. \quad (12)$$

Proof. Consider an integral

$$\int_{H^d} u_i(\mathbf{x}) \frac{\partial u_i(\mathbf{x})}{\partial x_i} d\mathbf{x}. \quad (13)$$

Applying the Cauchy–Schwarz inequality we obtain the following result:

$$\left(\int_{H^d} u_i(\mathbf{x}) \frac{\partial u_i(\mathbf{x})}{\partial x_i} d\mathbf{x} \right)^2 \leq \int_{H^d} u_i^2(\mathbf{x}) d\mathbf{x} \cdot \int_{H^d} \left(\frac{\partial u_i(\mathbf{x})}{\partial x_i} \right)^2 d\mathbf{x}. \quad (14)$$

It is easy to prove that the left and right parts of this inequality cannot be equal. Indeed, for them to be equal functions $u_i(\mathbf{x})$ and $\frac{\partial u_i(\mathbf{x})}{\partial x_i}$ should be linearly dependent. For simplicity consider a one-dimensional case: $x \in [0, 1]$. Let's assume

$$\frac{\partial u(x)}{\partial x} = Au(x),$$

where A is a constant. The general solution to this equation $u(x) = B \exp(Ax)$, where B is a constant. It is easy to see that this solution is not consistent with condition (3) which should be imposed on function $u(x)$.

Integral $\int_{H^d} u_i(\mathbf{x}) \frac{\partial u_i(\mathbf{x})}{\partial x_i} d\mathbf{x}$ can be transformed as

$$\begin{aligned}
\int_{H^d} u_i(\mathbf{x}) \frac{\partial u_i(\mathbf{x})}{\partial x_i} d\mathbf{x} &= \frac{1}{2} \int_{H^d} \frac{\partial u_i^2(\mathbf{x})}{\partial x_i} d\mathbf{x} \\
&= \frac{1}{2} \int_{H^{d-1}} (u_i^2(1, \mathbf{z}) - u_i^2(0, \mathbf{z})) d\mathbf{z} \\
&= \frac{1}{2} \int_{H^{d-1}} (u_i(1, \mathbf{z}) - u_i(0, \mathbf{z})) (u_i(1, \mathbf{z}) + u_i(0, \mathbf{z})) d\mathbf{z} \\
&= \frac{1}{2} \int_{H^d} (f(1, \mathbf{z}) - f(0, \mathbf{z})) (f(1, \mathbf{z}) + f(0, \mathbf{z}) - 2v(\mathbf{z})) d\mathbf{z}.
\end{aligned} \tag{15}$$

All terms in the last integrand are independent of x_i , hence we can replace integration with respect to $d\mathbf{z}$ to integration with respect to $d\mathbf{x}$ and substitute $v(\mathbf{z})$ for $f(\mathbf{x})$ in the integrand due to condition (3). Then (15) can be presented as

$$\int_{H^d} u_i(\mathbf{x}) \frac{\partial u_i(\mathbf{x})}{\partial x_i} d\mathbf{x} = \frac{1}{2} \int_{H^d} [f(1, \mathbf{z}) - f(0, \mathbf{z})] [f(1, \mathbf{z}) + f(0, \mathbf{z}) - 2f(\mathbf{x})] d\mathbf{x} \tag{16}$$

From (11) $\frac{\partial u_i(\mathbf{x})}{\partial x_i} = \frac{\partial f(\mathbf{x})}{\partial x_i}$, hence the right hand side of (14) can be written as $v_i D_i^{tot}$. Finally dividing (14) by $v_i D$ and using (16), we obtain the lower bound (12). \square

We call

$$\frac{(\int_{H^d} [f(1, \mathbf{z}) - f(0, \mathbf{z})] [f(1, \mathbf{z}) + f(0, \mathbf{z}) - 2f(\mathbf{x})] d\mathbf{x})^2}{4v_i D}$$

the lower bound number one (LB1).

Theorem 3. *There exists the following lower bound between DGSM (9) and the Sobol' total sensitivity index*

$$\frac{(2m+1) \left[\int_{H^d} (f(1, \mathbf{z}) - f(\mathbf{x})) d\mathbf{x} - w_i^{(m+1)} \right]^2}{(m+1)^2 D} < S_i^{tot} \tag{17}$$

Proof. Consider an integral

$$\int_{H^d} x_i^m u_i(\mathbf{x}) d\mathbf{x}. \tag{18}$$

Applying the Cauchy–Schwarz inequality we obtain the following result:

$$\left(\int_{H^d} x_i^m u_i(\mathbf{x}) d\mathbf{x} \right)^2 \leq \int_{H^d} x_i^{2m} d\mathbf{x} \cdot \int_{H^d} u_i^2(\mathbf{x}) d\mathbf{x}. \tag{19}$$

It is easy to see that equality in (19) cannot be attained. For this to happen functions $u_i(\mathbf{x})$ and x_i^m should be linearly dependent. For simplicity consider a one-dimensional case: $x \in [0, 1]$. Let's assume

$$u(x) = Ax^m,$$

where $A \neq 0$ is a constant. This solution does not satisfy condition (3) which should be imposed on function $u(x)$.

Further we use the following transformation:

$$\int_{H^d} \frac{\partial(x_i^{m+1} u_i(\mathbf{x}))}{\partial x_i} d\mathbf{x} = (m+1) \int_{H^d} x_i^m u_i(\mathbf{x}) d\mathbf{x} + \int_{H^d} x_i^{m+1} \frac{\partial u_i(\mathbf{x})}{\partial x_i} d\mathbf{x}$$

to present integral (18) in a form:

$$\begin{aligned} \int_{H^d} x_i^m u_i(\mathbf{x}) d\mathbf{x} &= \frac{1}{m+1} \left[\int_{H^d} \frac{\partial(x_i^{m+1} u_i(\mathbf{x}))}{\partial x_i} d\mathbf{x} - \int_{H^d} x_i^{m+1} \frac{\partial u_i(\mathbf{x})}{\partial x_i} d\mathbf{x} \right] \\ &= \frac{1}{m+1} \left[\int_{H^{d-1}} u_i(1, \mathbf{z}) d\mathbf{z} - \int_{H^d} x_i^{m+1} \frac{\partial u_i(\mathbf{x})}{\partial x_i} d\mathbf{x} \right] \\ &= \frac{1}{m+1} \left[\int_{H^d} (f(1, \mathbf{z}) - f(\mathbf{x})) d\mathbf{x} - \int_{H^d} x_i^{m+1} \frac{\partial u_i(\mathbf{x})}{\partial x_i} d\mathbf{x} \right]. \end{aligned} \quad (20)$$

We notice that

$$\int_{H^d} x_i^{2m} d\mathbf{x} = \frac{1}{(2m+1)}. \quad (21)$$

Using (20) and (21) and dividing (19) by D we obtain (17). \square

This second lower bound on S_i^{tot} we denote $\gamma(m)$:

$$\gamma(m) = \frac{(2m+1) \left[\int_{H^d} (f(1, \mathbf{z}) - f(\mathbf{x})) d\mathbf{x} - w_i^{(m+1)} \right]^2}{(m+1)^2 D} < S_i^{tot}. \quad (22)$$

In fact, this is a set of lower bounds depending on parameter m . We are interested in the value of m at which $\gamma(m)$ attains its maximum. Further we use star to denote such a value m : $m^* = \arg \max(\gamma(m))$ and call

$$\gamma^*(m^*) = \frac{(2m^*+1) \left[\int_{H^d} (f(1, \mathbf{z}) - f(\mathbf{x})) d\mathbf{x} - w_i^{(m^*+1)} \right]^2}{(m^*+1)^2 D} \quad (23)$$

the lower bound number two (LB2).

We define the maximum lower bound LB^* as

$$LB^* = \max(LB1, LB2). \quad (24)$$

We note that both lower and upper bounds can be estimated by a set of derivative based measures:

$$Y_i = \{v_i, w_i^{(m)}\}, m > 0. \quad (25)$$

3.2 Upper bounds on S_i^{tot}

Theorem 4.

$$S_i^{tot} \leq \frac{v_i}{\pi^2 D}. \quad (26)$$

The proof of this Theorem is given in [15].

Consider the set of values v_1, \dots, v_n , $1 \leq i \leq n$. One can expect that smaller v_i correspond to less influential variables x_i .

We further call (26) the upper bound number one (UB1).

Theorem 5.

$$S_i^{tot} \leq \frac{\varsigma_i}{D}, \quad (27)$$

where ς_i is given by (10).

Proof. We use the following inequality [2]:

$$0 \leq \int_0^1 u^2 dx - \left(\int_0^1 u dx \right)^2 \leq \frac{1}{2} \int_0^1 x(1-x)u'^2 dx. \quad (28)$$

The inequality is reduced to an equality only if u is constant. Assume that u is given by (3), then $\int_0^1 u dx = 0$, and from (28) we obtain (27). \square

Further we call $\frac{\varsigma_i}{D}$ the upper bound number two (UB2). We note that $\frac{1}{2}x_i(1-x_i)$ for $0 \leq x_i \leq 1$ is bounded: $0 \leq \frac{1}{2}x_i(1-x_i) \leq \frac{1}{8}$. Therefore, $0 \leq \varsigma_i \leq \frac{1}{8}v_i$.

3.3 Computational costs

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

In the case of straightforward numerical estimations of all partial derivatives 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 $f(0, z), f(1, z)$, while computing LB2 requires only values of $f(1, z)$. In total, numerical computation of LB^* for all input variables would require $N_F^{LB^*} = N(d+1) + 2Nd = N(3d+1)$ function evaluations. Computation of all upper bounds require $N_F^{UB} = N(d+1)$ function evaluations. We recall that the number of function evaluations required for computation of S_i^{tot} is $N_F^S = N(d+1)$ [10]. 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. The numerical efficiency of the DGSM method can be significantly increased by using algorithmic differentiation in the adjoint (reverse) mode [1]. This approach allows estimating all derivatives at a cost at most 6 times of that for evaluating the original function $f(x)$ [4]. However, as mentioned above lower bounds also require computation of $f(0, z), f(1, z)$ so $N_F^{LB^*}$ would only be reduced to $N_F^{LB^*} = 6N + 2Nd = N(2d+6)$, while N_F^{UB} would be equal to $6N$.

4 DGSM for random variables

Consider a function $f(x_1, \dots, x_d)$, where x_1, \dots, x_d are independent random variables with distribution functions $F_1(x_1), \dots, F_d(x_d)$. Thus the point $\mathbf{x} = (x_1, \dots, x_d)$ is defined in the Euclidean space R^d and its measure is $dF_1(x_1) \cdots dF_d(x_d)$.

The following DGSM was introduced in [15]:

$$v_i = \int_{R^d} \left(\frac{\partial f(\mathbf{x})}{\partial x_i} \right)^2 dF(\mathbf{x}). \quad (29)$$

We introduce a new measure

$$w_i = \int_{R^d} \frac{\partial f(\mathbf{x})}{\partial x_i} dF(\mathbf{x}). \quad (30)$$

4.1 The lower bounds on S_i^{tot} for normal variables

Assume that x_i is normally distributed with the finite variance σ_i^2 and the mean value μ_i .

Theorem 6.

$$\frac{\sigma_i^2 w_i^2}{D} \leq S_i^{tot}. \quad (31)$$

Proof. Consider $\int_{R^d} x_i u_i(\mathbf{x}) dF(\mathbf{x})$. Applying the Cauchy–Schwarz inequality we obtain

$$\left(\int_{R^d} x_i u_i(\mathbf{x}) dF(\mathbf{x}) \right)^2 \leq \int_{R^d} x_i^2 dF(\mathbf{x}) \cdot \int_{R^d} u_i^2(\mathbf{x}) dF(\mathbf{x}). \quad (32)$$

Equality in (32) can be attained if functions $u_i(\mathbf{x})$ and x_i are linearly dependent. For simplicity consider a one-dimensional case. Let's assume

$$u(x) = A(x - \mu),$$

where $A \neq 0$ is a constant. This solution satisfies condition (3) for normally distributed variable x with the mean value μ : $\int_{R^d} u(x) dF(x) = 0$.

For normally distributed variables the following equality is true [2]:

$$\left(\int_{R^d} x_i u_i(\mathbf{x}) dF(\mathbf{x}) \right)^2 = \int_{R^d} x_i^2 dF(\mathbf{x}) \cdot \int_{R^d} \frac{\partial u_i(\mathbf{x})}{\partial x_i} dF(\mathbf{x}). \quad (33)$$

By definition $\int_{R^d} x_i^2 dF(\mathbf{x}) = \sigma_i^2$. Using (32) and (33) and dividing the resulting inequality by D we obtain the lower bound (31). \square

4.2 The upper bounds on S_i^{tot} for normal variables

The following Theorem 7 is a generalization of Theorem 1.

Theorem 7. Assume that $c \leq \left| \frac{\partial f}{\partial x_i} \right| \leq C$, then

$$\frac{\sigma_i^2 c^2}{D} \leq S_i^{tot} \leq \frac{\sigma_i^2 C^2}{D}. \quad (34)$$

The constant factor σ_i^2 cannot be improved.

Theorem 8.

$$S_i^{tot} \leq \frac{\sigma_i^2}{D} v_i. \quad (35)$$

The constant factor σ_i^2 cannot be reduced.

Proofs are presented in [15].

5 Test cases

In this section we present the results of analytical and numerical estimation of S_i , S_i^{tot} , LB1, LB2 and UB1, UB2. The analytical values for DGSM and S_i^{tot} were calculated and compared with numerical results. For test case 2 we present convergence plots in the form of root mean square error (RMSE) versus the number of sampled points N . To reduce the scatter in the error estimation the values of RMSE were averaged over $K = 25$ independent runs:

$$\varepsilon_i = \left(\frac{1}{K} \sum_{k=1}^K \left(\frac{I_{i,k}^* - I_0}{I_0} \right)^2 \right)^{\frac{1}{2}}.$$

Here I_i^* is numerically computed values of S_i^{tot} , LB1, LB2 or UB1, UB2, I_0 is the corresponding analytical value of S_i^{tot} , LB1, LB2 or UB1, UB2. The RMSE can be approximated by a trend line $cN^{-\alpha}$. Values of $(-\alpha)$ are given in brackets on the plots. QMC integration based on Sobol' sequences was used in all numerical tests.

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

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

For this function $S_i = S_i^{tot}$, $D_i^{tot} = \frac{1}{12} \int_{H^{d-1}} a^2(z) dz$, $v_i = \int_{H^{d-1}} a^2(z) dz$, $LB1 = \frac{(\int_{H^d} (a^2(z) - 2a^2(z)x_i) dz dx_i)^2}{4D \int_{H^{d-1}} a^2(z) dz} = 0$ and $\gamma(m) = \frac{(2m+1)m^2 (\int_{H^{d-1}} a(z) dz)^2}{4(m+2)^2(m+1)^2 D}$. A maximum value

of $\gamma(m)$ is attained at $m^*=3.745$, when $\gamma^*(m^*) = \frac{0.0401}{D} (\int a(z) dz)^2$. The lower and upper bounds are $LB* \approx 0.48S_i^{tot}$. $UB1 \approx 1.22S_i^{tot}$. $UB2 = \frac{1}{12D} \int_0^1 a(z)^2 dz = S_i^{tot}$. For this test function $UB2 < UB1$.

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

$$f(\mathbf{x}) = \prod_{i=1}^d g_i,$$

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

Table 1 The analytical expressions for S_i , S_i^{tot} and $LB2$ for g-function

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

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

Table 2 The analytical expressions for S_i^{tot} , $UB1$ and $UB2$ for g-function

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

For this test function $\frac{S_i^{tot}}{UB1} = \frac{\pi^2}{48}$, $\frac{S_i^{tot}}{UB2} = \frac{1}{4}$, hence $\frac{UB2}{UB1} = \frac{\pi^2}{12} < 1$. Values of S_i , S_i^{tot} , UB and $LB2$ for the case of $a=[0,1,4.5,9,99,99,99,99]$, $d=8$ are given in Table 3 and shown in Figure 1. We can conclude that for this test function the knowledge of $LB2$ and $UB1$, $UB2$ allows to rank correctly all the variables in the order of their importance.

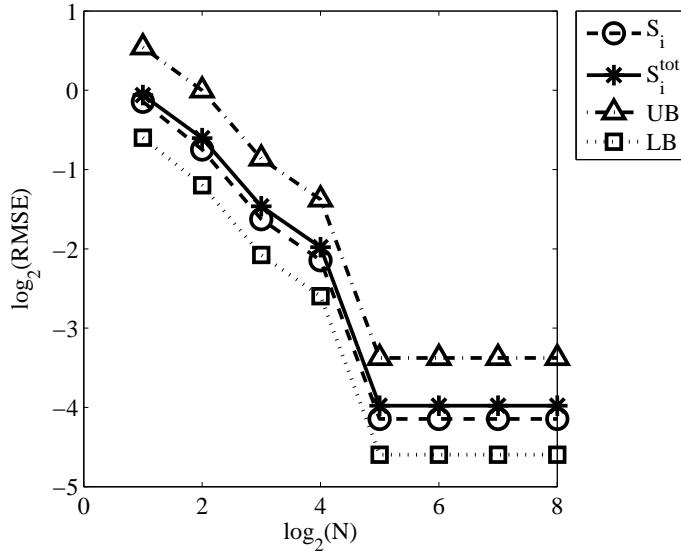


Fig. 1 Values of S_i, S_i^{tot} , LB2 and UB1 for all input variables. Example 2, $\alpha=[0,1,4.5,9,99,99,99], d=8$.

Fig. 2 presents RMSE of numerical estimations of S_i^{tot} , UB1 and LB2. For an individual input LB2 has the highest convergence rate, following by S_i^{tot} , and UB1 in terms of the number of sampled points. However, we recall that computation of all indices requires $N_F^{LB*} = N(3d + 1)$ function evaluations for LB, while for S_i^{tot} this number is $N_F^S = N(d + 1)$ and for UB it is also $N_F^{UB} = N(d + 1)$.

Example 3. Hartmann function $f(\mathbf{x}) = -\sum_{i=1}^4 c_i \exp \left[-\sum_{j=1}^n \alpha_{ij}(x_j - p_{ij})^2 \right]$, $x_i \in [0, 1]$. For this test case a relationship between the values LB1, LB2 and S_i varies with the change of input (Table 4, Figure 3): for variables x_2 and x_6 $LB1 > S_i > LB2$, while for all other variables $LB1 < LB2 < S_i$. LB^* is much smaller than S_i^{tot} for all inputs. Values of m^* also vary with the change of input. For all variables but variable 2 UB1 > UB2.

Table 3 Values of LB^* , S_i , S_i^{tot} , UB1 and UB2. Example 2, $\alpha=[0,1,4.5,9,99,99,99], d=8$.

	x_1	x_2	x_3	x_4	$x_5 \dots x_8$
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	0.000501
$UB2$	3.149	0.969	0.137	0.0418	0.00042

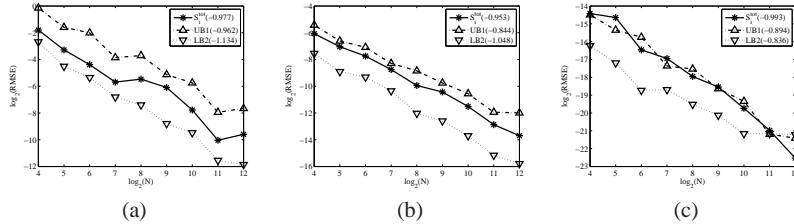


Fig. 2 RMSE of S_i^{tot} , UB and LB2 versus the number of sampled points. Example 2, $a=[0,1,4.5,9,99,99,99,99]$, $d=8$. Variable 1 (a), variable 3 (b) and variable 5 (c).

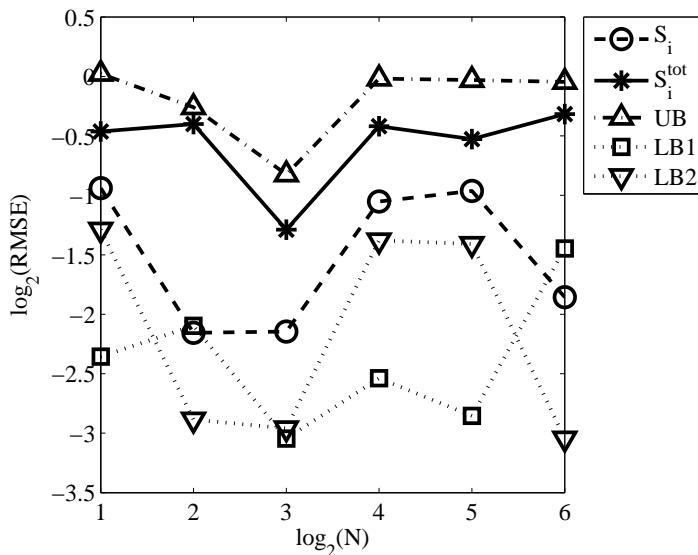


Fig. 3 Values of S_i, S_i^{tot} , UB1, LB1 and LB2 for all input variables. Example 3.

Table 4 Values of m^* , LB1, LB2, UB1, UB2, S_i and S_i^{tot} for all input variables.

	x_1	x_2	x_3	x_4	x_5	x_6
$LB1$	0.0044	0.0080	0.0009	0.0029	0.0014	0.0357
$LB2$	0.0515	0.0013	0.0011	0.0418	0.0390	0.0009
m^*	4.6	10.2	17.0	5.5	3.6	19.9
LB^*	0.0515	0.0080	0.0011	0.0418	0.0390	0.0357
S_i	0.115	0.00699	0.00715	0.0888	0.109	0.0139
S_i^{tot}	0.344	0.398	0.0515	0.381	0.297	0.482
$UB1$	1.089	0.540	0.196	1.088	1.073	1.046
$UB2$	1.051	0.550	0.150	0.959	0.932	0.899

6 Conclusions

We can conclude that using lower and upper bounds based on DGSM it 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} . Small values of upper bounds imply small values of S_i^{tot} . DGSM can be used for fixing unimportant variables and subsequent model reduction. For linear function and product function, DGSM can give the same variable ranking as S_i^{tot} . In a general case variable ranking can be different for DGSM and variance based methods. Upper and lower bounds can be estimated using MC/QMC integration methods using the same set of partial derivative values. Partial derivatives can be efficiently estimated using algorithmic differentiation in the reverse (adjoint) mode.

We note that all bounds should be computed with sufficient accuracy. Standard techniques for monitoring convergence and accuracy of MC/QMC estimates should be applied to avoid erroneous results.

Acknowledgements The authors would like to thank Prof. I. Sobol' his invaluable contributions to this work. Authors also gratefully acknowledge the financial support by the EPSRC grant EP/H03126X/1.

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