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Monte Carlo evaluation of derivative-based global sensitivity measures

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ABSTRACT

A novel approach for evaluation of derivative-based global sensitivity measures (DGSM) is presented. It is compared with the Morris and the Sobol' sensitivity indices methods. It is shown that there is a link between DGSM and Sobol' sensitivity indices. DGSM are very easy to implement and evaluate numerically. The computational time required for numerical evaluation of DGSM is many orders of magnitude lower than that for estimation of the Sobol' sensitivity indices. It is also lower than that for the Morris method. Efficiencies of Monte Carlo (MC) and quasi-Monte Carlo (QMC) sampling methods for calculation of DGSM are compared. It is shown that the superiority of QMC over MC depends on the problem's effective dimension, which can also be estimated using DGSM.

1. Introduction

Sensitivity analysis (SA) is widely used in engineering design. One of the widespread SA approaches is based on local methods. Local SA techniques are usually concerned with the computation of the derivative of the model response with respect to the model input parameters. The main disadvantage of these methods is that they do not account for interactions between variables and the local sensitivity coefficients are related to a fixed nominal point in the space of parameters.

Global 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 [1,2]. The method of global sensitivity indices suggested by Sobol' in [3], and then further developed by Saltelli and Sobol' in [4], Homma and Saltelli in [5] 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. Variance-based methods generally require a large number of function evaluations to achieve reasonable convergence and can become impractical for large engineering problems. This is why a number of alternative SA techniques have been proposed recently. One of them is the screening method proposed by Morris [6]. 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 ranking and 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 cannot 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 uncertainly) and it cannot distinguish between low-and high-order interactions.

In this paper, we present a new method, which we call derivative-based global sensitivity measures (DGSM). The method is based on averaging local derivatives using Monte Carlo (MC) or quasi-Monte Carlo (QMC) 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 with 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. We also introduce new sensitivity measures and demonstrate that there is a link between these measures and the Sobol' sensitivity indices.

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It is well known that for a sufficiently large number of sampled points N, QMC should always outperform MC [7]. However, for high-dimensional problems such a large number of points can be infeasible. Some numerical experiments demonstrated that the advantages of QMC integration can disappear for high-dimensional problems. At the same time there are high-dimensional problems for which QMC remains more efficient than MC. It was shown that the Sobol' method can be used for the prediction of the QMC efficiency [8]. In this paper, we show that DGSM can also be used as quantitative measures of the QMC efficiency.

This paper is organised as follows: Section 2 introduces DGSM. Section 3 gives a brief description of Sobol' global sensitivity indices. MC and QMC integration algorithms and low-discrepancy sequences are discussed in Section 4. This section also contains a description of the DGSM algorithm. Section 5 briefly describes the Morris method. Section 6 covers issues concerning the possible degradation of QMC efficiency in higher dimensions. It also introduces the notion of the effective dimension and presents the classification of functions based on Sobol' global sensitivity indices. It is shown how this classification can be used for the prediction of the QMC efficiency. A comparison of the Sobol' method, DGSM and the Morris methods is given in Section 7. Finally, conclusions are presented in Section 8.

2. Derivative-based global sensitivity measures

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

$$E_i(x^*)=\frac{\partial f}{\partial x_i}. \tag{1}$$

The local sensitivity measure $E_i(x^*)$ depends on a nominal point x^* and it changes with a change of x^*. This deficiency can be overcome by averaging $E_i(x^*)$ over the parameter space H^n. Such a measure can be defined as

$$\bar{M}_i=\int_{H^n} E_i\,\mathrm{d}x. \tag{2}$$

We also consider another measure, which is the standard deviation of E_i

$$\bar{\Sigma}_i=\left[\int_{H^n}(E_i-\bar{M}_i)^2\,\mathrm{d}x\right]^{1/2}. \tag{3}$$

$\bar{\Sigma}_i$ can also be presented as

$$\bar{\Sigma}_i^2=\int_{H^n} E_i^2\,\mathrm{d}x-\bar{M}_i^2.$$

Combining $\bar{M}_i$ and $\bar{\Sigma}_i$ a new measure can be introduced

$$\bar{\Sigma}_i^2+\bar{M}_i^2=\int_{H^n} E_i^2\,\mathrm{d}x. \tag{4}$$

Measure

$$\bar{G}_s=\frac{\sum_{i=1}^{s} G_i}{\sum_{i=1}^{n} G_i}, \tag{5}$$

where $G_i=\bar{\Sigma}_i^2+\bar{M}_i^2$, s is a number of variables in a subset was considered in [9]. It was called there an "alternative global sensitivity estimator".

From (4) we can obtain a ratio

$$\bar{M}_i/\bar{\Sigma}_i=\left(1/\bar{\Sigma}_i^2\int_{H^n} E_i^2\,\mathrm{d}x-1\right)^{1/2}. \tag{6}$$

Non-monotonic functions have regions of positive and negative values of partial derivatives $E_i(x^*)$, hence due to the effect of averaging values of $\bar{M}_i$ can be very small or even zero: e.g. for a symmetrical at a middle point $x=0.5$ function $\bar{M}_i=0$. To avoid the cancelling effect, measures based on the absolute value of $|E_i(x^*)|$ can be used

$$\bar{M}_i^*=\int_{H^n}|E_i|\,\mathrm{d}x, \tag{7}$$

$$\bar{\Sigma}_i^*=\left[\int_{H^n}(|E_i|-\bar{M}_i^*)^2\,\mathrm{d}x\right]^{1/2}. \tag{8}$$

Similar measures were introduced in [10] within the framework of the Morris method. It is clear from the definition of G_i (5) that the cancelling effect does not affect the values of this measure.

Using an analogy with variance-based global sensitivity measures, we call the set of measures $\bar{M}_i$, $\bar{\Sigma}_i$ and $\bar{G}_i$ DGSM.

3. Sobol' global sensitivity indices

The method of global sensitivity indices developed by Sobol' is based on ANOVA decomposition [3]. Consider a square integrable function $f(x)$ defined in the unit hypercube H^n. It can be expanded in the following form:

$$f(x)=f_0+\sum_i f_i(x_i)+\sum_{i<j} f_{ij}(x_i,x_j)+\cdots+f_{12\ldots n}(x_1,x_2,\ldots,x_n). \tag{9}$$

This decomposition is unique if conditions

$$\int_0^1 f_{i_1\ldots i_s}\,\mathrm{d}x_{i_k}=0 \quad \text{for } 1\leqslant k\leqslant s,$$

are satisfied. Here $1\leqslant i_1<\cdots<i_s\leqslant n$. It follows from (9) and (10) that

$$f_0=\int_0^1 f(x)\,\mathrm{d}x.$$

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

$$D=\sum_{s=1}^{n}\sum_{i_1<\cdots<i_s}^{n} D_{i_1\ldots i_s},$$

where $D_{i_1\ldots i_s}=\int_0^1 f_{i_1\ldots i_s}^2(x_{i_1},\ldots,x_{i_s})\,\mathrm{d}x_{i_1},\ldots,x_{i_s}$ are called partial variances.

Sobol' defined the global sensitivity indices as the ratios

$$S_{i_1\ldots i_s}=D_{i_1\ldots i_s}/D. \tag{10}$$

All $S_{i_1\ldots i_s}$ are non-negative and add up to one

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

There are 2^n terms in this summation and calculation of all of them is not practical. For this reason Sobol' introduced sensitivity indices for subsets of variables. Consider two complementary subsets of variables y and z

$$x=(y,z).$$

Let $y=(x_{i_1},\ldots,x_{i_m}), 1\leqslant i_1<\cdots<i_m\leqslant n, K=(i_1,\ldots,i_m)$. The variance corresponding to a set y is defined as

$$D_y^2=\sum_{s=1}^{m}\sum_{(i_1<\cdots<i_s)\in K} D_{i_1\ldots i_s}^2. \tag{11}$$

$D_y{}^2$ includes all partial variances $D_{i_1}^2, D_{i_2}^2,\ldots,D_{i_1\ldots i_s}^2$, such that their subsets of indices $(i_1,\ldots,i_s)\in K$.

The total sensitivity indices were introduced by Homma and Saltelli in [5]. The total variance $(D_y{}^{\mathrm{T}})^2$ is defined as

$$(D_y^{\mathrm{T}})^2=D^2-D_z^2$$

$(D_y^{\mathrm{T}})^2$ consists of all $D^2_{i_1\ldots i_s}$ 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

$$S_y = D_y^2/D^2,$$
$$S_y^{\mathrm{T}} = (D_y^{\mathrm{T}})^2/D^2. \quad (12)$$

$S_y^{\mathrm{T}} = 1 - S_z$. The difference $S_y^{\mathrm{T}} - S_y$ accounts for all interactions between y and z.

The important indices in practice are S_i and S_i^{T}. Their values in most cases provides sufficient information to determine the sensitivity of the analysed function to individual input variables. As shown in Section 6, they can also be used to classify functions in respect of efficiencies of MC and QMC integrations.

4. Computational algorithms for calculation of derivative-based global sensitivity measures

Calculation of DGSM is based on the evaluation of integrals (2)–(8), which can be presented in the following generic form:

$$I[f] = \int_{H^n} f(x)\,\mathrm{d}x. \quad (13)$$

It is assumed that function $f(x)$ is integrable in the n-dimensional unit hypercube H^n.

Classical grid methods become inefficient in high dimensions because of the "curse of dimensionality" (exponential growth of the required integrand evaluations). MC methods do not depend on the dimensionality and are effective in high-dimensional integrations. The MC quadrature formula is based on the probabilistic interpretation of an integral. For a random variable that is uniformly distributed in H^n

$$I[f] = E[f(x)],$$

where $E[f(x)]$ is the mathematical expectation. An approximation to this expectation is

$$I_N[f] = \frac{1}{N}\sum_{i=1}^{N} f(x_i), \quad (14)$$

Table 3
Test functions and their classification

Function	$f(x)$
A1	$\sum_{i=1}^{n}(-1)^i \prod_{j=1}^{i} x_j$
A2	$\prod_{i=1}^{n} \frac{\lvert 4x_i-2\rvert + a_i}{1+a_i}, a_1 = a_2 = 0, a_3 = \ldots = a_n = 6.52$
B1	$\prod_{i=1}^{n} \frac{n-x_i}{n-0.5}$
B2	$\prod_{i=1}^{n} \frac{\lvert 4x_i-2\rvert + a_i}{1+a_i}, a_i = 50$
C1	$2^n \prod_{i=1}^{n} x_i$
C2	$\prod_{i=1}^{n} \lvert 4x_i - 2\rvert$
A3	$\sum_{i=1}^{4} \beta_i w_i + \sum_{i\leqslant j}^{4} \beta_{ij} w_i w_j + \sum_{i\leqslant j\leqslant k}^{4} \beta_{ijk} w_i w_j w_k$

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

Table 4
Analytical values for indices S_i, S_i^{T} and the ratio S_i/S_i^{T} for function A1

x_i	S_i	S_i^{T}	S_i/S_i^{T}
1	0.67	0.75	0.89
2	0.17	0.25	0.68
3	4.1×10^{-2}	8.3×10^{-2}	0.49
4	1.0×10^{-2}	2.8×10^{-2}	0.36
5	2.5×10^{-3}	9.2×10^{-3}	0.27
6	6.9×10^{-4}	3.2×10^{-3}	0.21
7	1.4×10^{-4}	9.3×10^{-4}	0.15
8	5.1×10^{-5}	4.2×10^{-4}	0.12
9	5.7×10^{-6}	7.6×10^{-5}	0.075
10	5.7×10^{-6}	7.6×10^{-5}	0.075

Table 1
Classification of functions based on Sobol' sensitivity indices

Function type	Description	Relationship between S_i and S_i^{T}	d_{T}	d_S	QMC is more efficient than MC
A	A few dominant variables	$S_y^{\mathrm{T}}/n_y \gg S_z^{\mathrm{T}}/n_z$	$\ll n$	$< n$	Yes
B	No unimportant subsets; Important low-order interaction terms	$S_i \approx S_j, \forall i,j$ $S_i/S_j^{\mathrm{T}} \approx 1, \forall i$	$\approx n$	$\ll n$	Yes
C	No unimportant subsets; Important high-order interaction terms	$S_i \approx S_j, \forall i,j$ $S_i/S_j^{\mathrm{T}} \ll 1, \forall i$	$\approx n$	$\approx n$	No

Table 2
Classification of functions based on DGSM

Function type	Description	Relationship between S_i and S_i^{T}	d_{T}	d_S	QMC is more efficient than MC
A	A few dominant variables	$\frac{\sum_{i=1}^{d_{\mathrm{T}}} G_{i_i}}{n_y} \gg \frac{\sum_{i=d_{\mathrm{T}}+1}^{n} G_i}{n_z}$	$\ll n$	$< n$	Yes
B	No unimportant subsets; important low-order interaction terms	$\bar{M}_i^* \approx \bar{M}_j^*, \bar{\Sigma}_i^* \approx \bar{\Sigma}_j^*, \forall i,j$ $\bar{M}_i^*/\bar{\Sigma}_i^* \geqslant 1, \forall i$	$\approx n$	$\ll n$	Yes
C	No unimportant subsets; important high-order interaction terms	$\bar{M}_i^* \approx \bar{M}_j^*, \bar{\Sigma}_i^* \approx \bar{\Sigma}_j^*, \forall i,j$ $\bar{M}_i^*/\bar{\Sigma}_i^* \ll 1, \forall i$	$\approx n$	$\approx n$	No

where $\{x_i\}$ is a sequence of random points in H^n of length N. The approximation $I_N[f]$ converges to $I[f]$ with probability 1.

Consider an integration error defined as

$$\varepsilon = |I[f] - I_N[f]|.$$

It follows from the Central Limit Theorem that the expectation of ε^2 is

$$E(\varepsilon^2) = \frac{\sigma^2(f)}{N},$$

where $\sigma^2(f)$ is the variance given by

$$\sigma^2(f) = \int_{H^n} f^2(x)\,dx - \left(\int_{H^n} f(x)\,dx\right)^2.$$

The root mean-square error (RMSE) of the MC method is

$$\varepsilon_N = (E(\varepsilon^2))^{1/2} = \frac{\sigma(f)}{N^{1/2}}.$$

The convergence rate of MC does not depend on the number of variables n although it is rather low.

The efficiency of MC methods is determined by the properties of random numbers. It is known that random number sampling is prone to clustering: for any sampling there are always empty areas as well as regions in which random points are wasted due to clustering. As new points are added randomly, they do not necessarily fill the gaps between already sampled points.

A higher rate of convergence can be obtained by using deterministic uniformly distributed sequences also known as low-discrepancy sequences (LDS) instead of pseudo-random numbers. Methods based on the usage of such sequences are known as QMC methods.

LDS are specifically designed to place sample points as uniformly as possible. Unlike random numbers, successive LDS points "know" about the position of previously sampled points and "fill" the gaps between them. LDS are also known as quasi-random numbers. The QMC algorithm for the evaluation of the integral (13) has a form similar to (14)

$$I_N = \frac{1}{N}\sum_{i=1}^{N} f(q_i). \tag{15}$$

Here $\{q_i\}$ is a set of LDS points uniformly distributed in a unit hypercube H^n, $q_i = q_i^1, \ldots, q_i^n$.

Table 5
Analytical values for $\bar{M}_i^*$, $\bar{\Sigma}_i^*$, $\bar{M}_i^*/\bar{\Sigma}_i^*$ and G_i for function A1

x_i	$\bar{M}_i^*$	$\bar{\Sigma}_i^*$	$\bar{M}_i^*/\bar{\Sigma}_i^*$	G_i
1	0.67	0.23	2.82	0.67
2	0.33	0.23	1.43	0.22
3	0.17	0.17	1.0	7.3×10^{-2}
4	8.4 × 10−2	0.11	0.76	2.5×10^{-2}
5	4.1×10^{-2}	6.6×10^{-2}	0.62	8.0×10^{-3}
6	2.1×10^{-2}	4.1×10^{-2}	0.51	2.9×10^{-3}
7	9.8×10^{-3}	2.3×10^{-2}	0.43	8.3×10^{-4}
8	5.9×10^{-3}	1.6×10^{-2}	0.37	3.7×10^{-4}
9	2.0×10^{-3}	6.9×10^{-3}	0.29	6.7×10^{-5}
10	2.0×10^{-3}	6.9×10^{-3}	0.29	6.7×10^{-5}

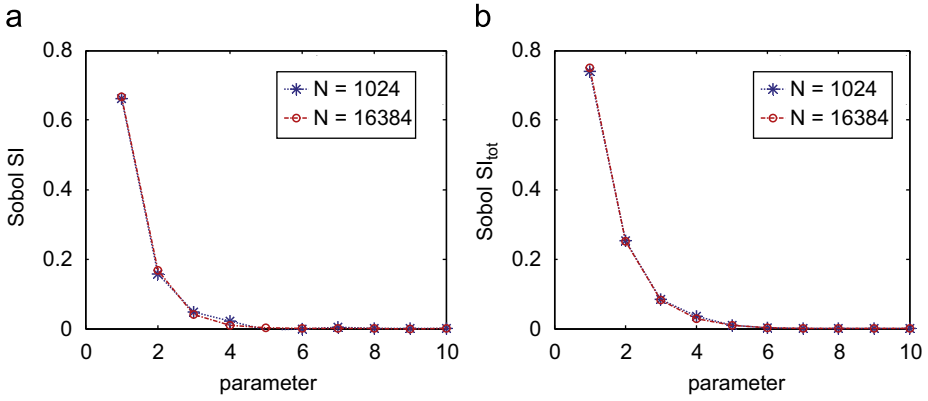

Fig. 1. Numerical evaluation of sensitivity indices S_i (a) and total sensitivity indices S_i^T (b) for A1 function at two different numbers of sampling points $N = 1024$ ($N_F = 12{,}288$) and $N = 16{,}384$ ($N_F = 196{,}608$).

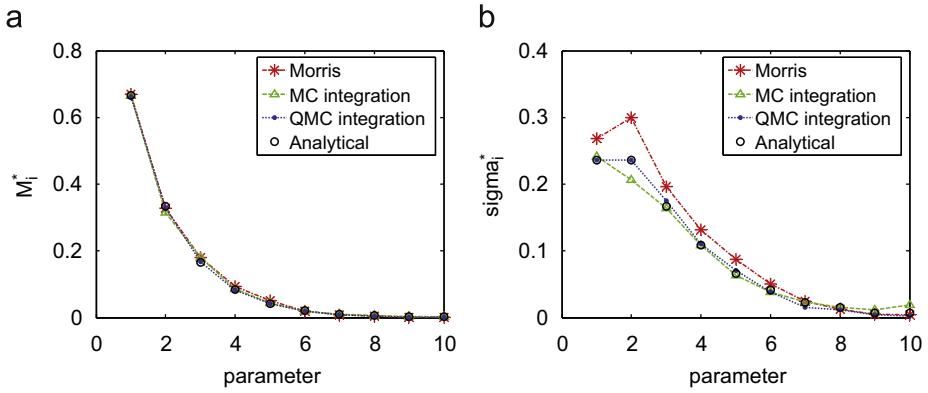

Fig. 2. Comparison of numerical evaluation of $\bar{M}_i^*$ (a) and $\bar{\Sigma}_i^*$ (b) with analytical values for A1 function by the Morris method and DGSM methods with MC and QMC integrations at number of function evaluations $N_F = 1408$.

There are a few well known and commonly used LDS. Different principles were used for their construction by Holton, Faure, Sobol', Niederreiter and others. Many practical studies have proven that the Sobol' LDS is in many aspects superior to other LDS [11–13]. For this reason it was used in this work.

For the best-known LDS the estimate for the rate of convergence $I_N \to I$ is known to be $O(\ln^n N)/N$. This rate of convergence is much faster than that for the MC method, although it depends on the dimensionality n.

Evaluation of DGSM measures requires calculation of $E_i(x^*)$ defined by formula (1). It can be done analytically for easily differentiable functions or numerically

$$E_i(x^*) = \frac{\left[f(x_1^*, \ldots, x_{i-1}^*, x_i^* + \delta, x_{i+1}^*, \ldots, x_n^*) - f(x^*)\right]}{\delta}. \quad (16)$$

Here δ is a small increment. The total number of function evaluations for calculation of a full set of $\{\bar{M}_i\}$, $\{\bar{\Sigma}_i\}$ and $\{\bar{G}_i\}$ is $N_F = N(n+1)$.

5. 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. It is composed of individually randomized 'one-factor-at-a-time' 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 [6] 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 ith input factor is defined as

$$EE_i(x^*) = \frac{\left[f(x_1^*, \ldots, x_{i-1}^*, x_i^* + \Delta, x_{i+1}^*, \ldots, x_n^*) - f(x^*)\right]}{\Delta}, \quad (17)$$

where Δ is a predetermined multiple of $1/(p-1)$ and point $x^* \in H^n$ is such that $x_i^* + \Delta \leqslant 1$. The distribution of elementary effects F_i is obtained by randomly sampling N points from H^n. Two sensitivity measures are evaluated for each factor: μ_i an estimate of the mean of the distribution F_i, and σ_i an estimate of the standard deviation of F_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 total computational cost for this method is $N_F = 2Nn$. However, it can be reduced. Morris suggested a more economical algorithm by using already computed values of functions in calculation of more than one elementary effect. His algorithm involves a calculation of the so-called sampling matrix, which is used for generating trajectories of n steps in the input variable space. These trajectories are such that on each step only one component of a starting point $x = (x_1, x_2, \ldots, x_n)$ taken from grid-levels is increased by Δ. The computational cost of the Morris method is $N_F = N(n+1)$. The revised version of the $EE_i(x^*)$ 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. [10].

Table 6
Ratios $\bar{M}_i^*/S_i^T$, G_i/S_i^T and $(\bar{M}_i^*/\bar{\Sigma}_i^*)/(S_i/S_i^T)$ for function A1

x_i	$\bar{M}_i^*/S_i^T$	G_i/S_i^T	$(\bar{M}_i^*/\bar{\Sigma}_i^*)/(S_i/S_i^T)$
1	0.89	0.89	3.16
2	1.32	0.89	2.10
3	2.05	0.89	2.04
4	3.0	0.89	2.11
5	4.46	0.89	2.29
6	6.46	0.89	2.42
7	10.54	0.89	2.86
8	14.05	0.89	3.08
9	26.23	0.89	3.86
10	26.23	0.89	3.86

Table 7
Analytical values for indices S_i, S_i^T and the ratio S_i/S_i^T for function A2

x_i	S_i	S_i^T	S_i/S_i^T
1	0.39	0.54	0.71
2	0.39	0.54	0.71
$i = 3$–10	6.9×10^{-3}	1.3×10^{-2}	0.55

Table 8
Analytical values for $\bar{M}_i^*$, $\bar{\Sigma}_i^*$, $\bar{M}_i^*/\bar{\Sigma}_i^*$ and G_i for function A2

x_i	$\bar{M}_i^*$	$\bar{\Sigma}_i^*$	$\bar{M}_i^*/\bar{\Sigma}_i^*$	G_i
1	4.0	2.52	1.59	0.50
2	4.0	2.52	1.59	0.50
$i = 3$–10	0.53	0.49	1.08	1.1×10^{-2}

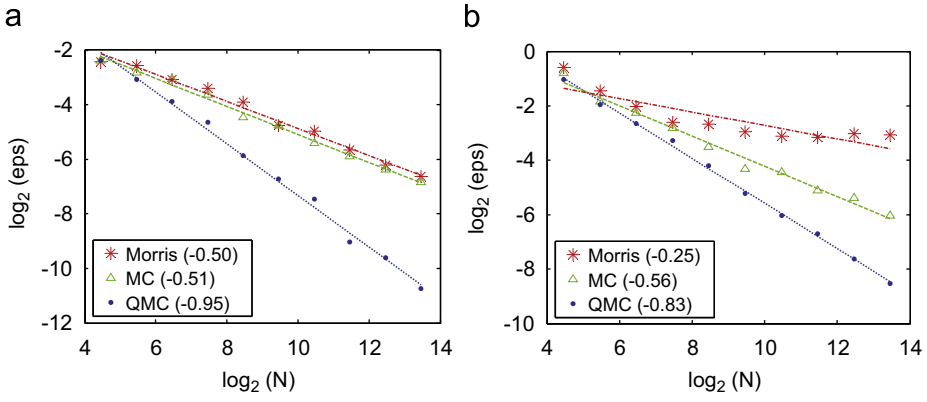

Fig. 3. The integration error of $\bar{M}_1^*$ (a) and $\bar{\Sigma}_1^*$ (b) evaluated by the Morris method and DGSM methods with MC and QMC integrations vs the number of sampled points N. A1 function.

For the reason given in Section 2, Campolongo et al. [10] considered another sensitivity measure μ_i^*, which is an estimate of the mean of the distribution of the absolute values of the elementary effects and showed that μ_i^* gives a better estimate of the order of importance than μ_i. It was also noticed that μ_i^* has similarities with S_i^T in that it gives a ranking of the variables very similar to that based on the S_i^T but no formal proof of the link between μ_i^* and S_i^T was given [1,10].

Table 9
Ratios $\bar{M}_i^*/S_i^T$, G_i/S_i^T and $(\bar{M}_i^*/\bar{\Sigma}_i^*)/(S_i/S_i^T)$ for function A2

x_i	$\bar{M}_i^*/S_i^T$	G_i/S_i^T	$(\bar{M}_i^*/\bar{\Sigma}_i^*)/(S_i/S_i^T)$
1	7.41	0.9	2.23
2	7.41	0.9	2.23
$i = 3$–10	40.77	0.9	1.96

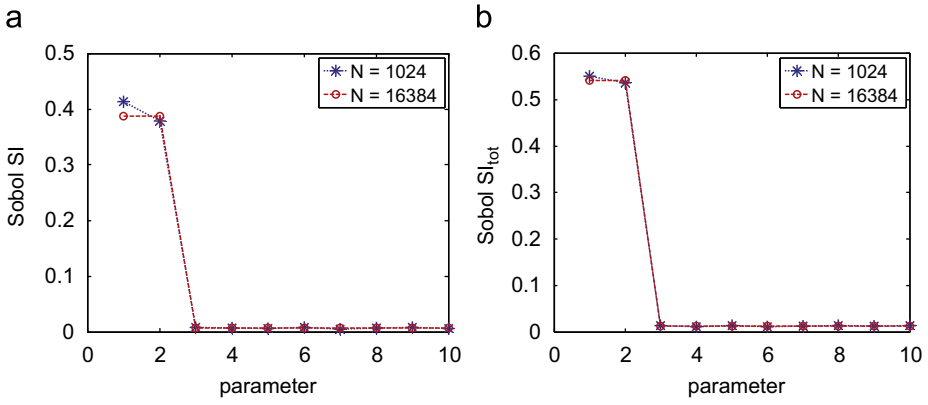

Fig. 4. Numerical evaluation of sensitivity indices S_i (a) and total sensitivity indices S_i^T (b) for A2 function at two different numbers of sampling points $N = 1024$ ($N_F = 12{,}288$) and $N = 16{,}384$ ($N_F = 196{,}608$).

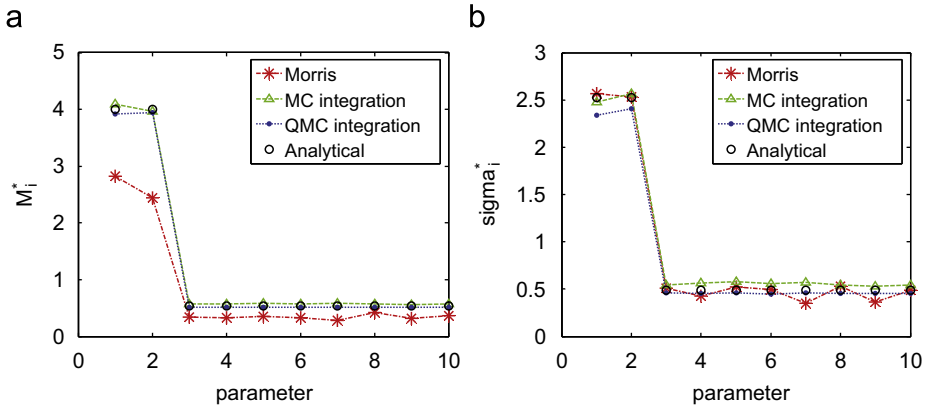

Fig. 5. Comparison of numerical evaluation of $\bar{M}_i^*$ (a) and $\bar{\Sigma}_i^*$ (b) for A2 function with analytical values by the Morris method and DGSM methods with MC and QMC integrations at number of function evaluations $N_F = 1408$.

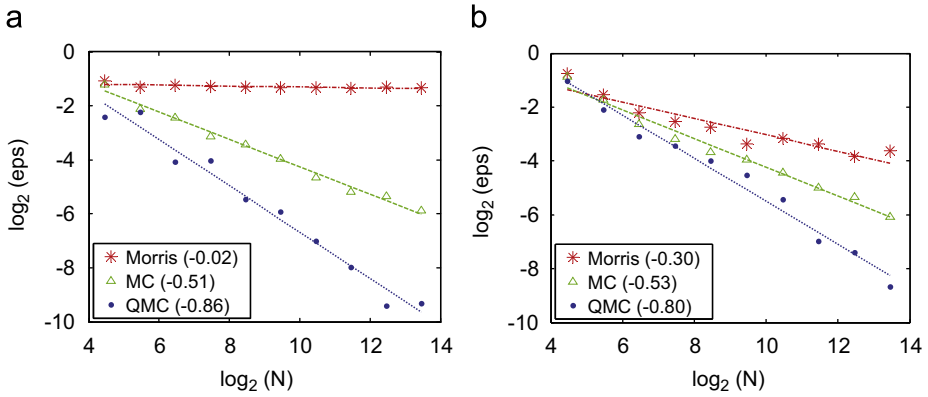

Fig. 6. The integration error of $\bar{M}_1^*$ (a) and $\bar{\Sigma}_1^*$ (b) evaluated by the Morris method and DGSM methods with MC and QMC integrations vs the number of sampled points *N*. A2 function.

6. The effective dimension and classification of test functions

Generally, QMC is much more efficient than MC. However, some numerical experiments demonstrated that the advantages of QMC integration can disappear for high-dimensional problems [11]. There are also high-dimensional problems for which QMC outperforms MC [12]. Such behaviour can be explained by the problem's effective dimension. The notion of the "effective dimension" was introduced by Caflisch et al. [14].

Let $|\mathbf{u}|$ be a cardinality of a set $\mathbf{u}$.

Definition 1. The effective dimension of $f(x)$ in the superposition sense is the smallest integer d_S such that

$$\sum_{0<|u|\leqslant d_s} S_u \geqslant (1-\varepsilon), \tag{18}$$

where ε is a small parameter, e.g. $\varepsilon \approx 0.01$. Here S_u denotes sensitivity index with indices from the set $\mathbf{u}$.

Condition (18) means that the function $f(x)$ is almost a sum of d_S-dimensional functions. The effective dimension d_S is the order of the highest effect one needs to include in the sum $\sum_{0<|u|\leqslant d_s} S_u$ in order to reach the $(1-\varepsilon)$ target.

Definition 2. The effective dimension in the truncation sense is the smallest integer d_T such that

$$\sum_{u\subseteq\{1,2,\ldots,d_T\}} S_u \geqslant (1-\varepsilon). \tag{19}$$

In other words, the effective dimension d_T is the highest number of factors, which need to be included in the sum $\sum_{u\subseteq\{1,2,\ldots,d_T\}} S_u$ in order to reach the $(1-\varepsilon)$ target.

The value d_S does not depend on the order in which the input variables are sampled, while d_T does. It was suggested in [14,15] that the efficiency of QMC methods on high-dimensional problems can be attributed to the low effective dimension of the integrand (in one or both of the senses).

A straightforward evaluation of the effective dimension in the superposition sense d_S from its definitions (18) is not practical in the general case as it would require the calculation of all 2^n sensitivity indices $S_{ij,\ldots,k}$.

Owen introduced the dimension distribution for a square integrable function [15]. The effective dimension can be defined through a quantile of the dimension distribution. Owen showed that the dimension distribution can be linked to the Sobol' sensitivity indices. Several cases of additive and multiplicative test functions were considered. For these types of functions quantiles of the dimension distribution can be explicitly calculated. However, they are difficult to estimate in a general case.

A ratio S_i/S_i^T, which will require the calculation of only $2n$ sensitivity indices can provide information about importance of high-order interactions: if $S_i/S_i^T \approx 1$, $\forall i$, then only main effects are present in the ANOVA decomposition (9) and hence $d_S \approx 1$. If $S_i/S_i^T < 1$ then $d_S > 1$ although an exact value of d_S would not be possible to establish from just the values of S_i and S_i^T and calculation of higher-order indices $S_{ij,\ldots,k}$. would also be required.

The effective dimension in the truncation sense d_T is somewhat easier to evaluate. Consider two complementary subsets of

Table 10
Analytical values for indices S_i, S_i^T and the ratio S_i/S_i^T for function B1

x_i	S_i	S_i^T	S_i/S_i^T
$i=1$–10	0.1	0.1	1.0

Table 11
Analytical values for $\tilde{M}_i^*$, $\tilde{\Sigma}_i^*$, $\tilde{M}_i^*/\tilde{\Sigma}_i^*$, $\sqrt{\tilde{M}_i^{*2}+\tilde{\Sigma}_i^{*2}}$ and G_i for function B1

x_i	$\tilde{M}_i^*$	$\tilde{\Sigma}_i^*$	$\tilde{M}_i^*/\tilde{\Sigma}_i^*$	$\sqrt{\tilde{M}_i^{*2}+\tilde{\Sigma}_i^{*2}}$	G_i
$i=$ 1–10	0.1	9.61×10^{-3}	10.4	0.11	0.1

Table 12
Analytical values for indices S_i, S_i^T and the ratio S_i/S_i^T for function B2

x_i	S_i	S_i^T	S_i/S_i^T
$I=1$–10	0.1	0.1	1.0

Table 13
Analytical values for $\tilde{M}_i^*$, $\tilde{\Sigma}_i^*$, $\tilde{M}_i^*/\tilde{\Sigma}_i^*$, $\sqrt{\tilde{M}_i^{*2}+\tilde{\Sigma}_i^{*2}}$ and G_i for function B2

x_i	$\tilde{M}_i^*$	$\tilde{\Sigma}_i^*$	$\tilde{M}_i^*/\tilde{\Sigma}_i^*$	$\sqrt{\tilde{M}_i^{*2}+\tilde{\Sigma}_i^{*2}}$	G_i
$i=1$–10	7.84×10^{-2}	2.66×10^{-3}	29.5	7.85×10^{-2}	0.1

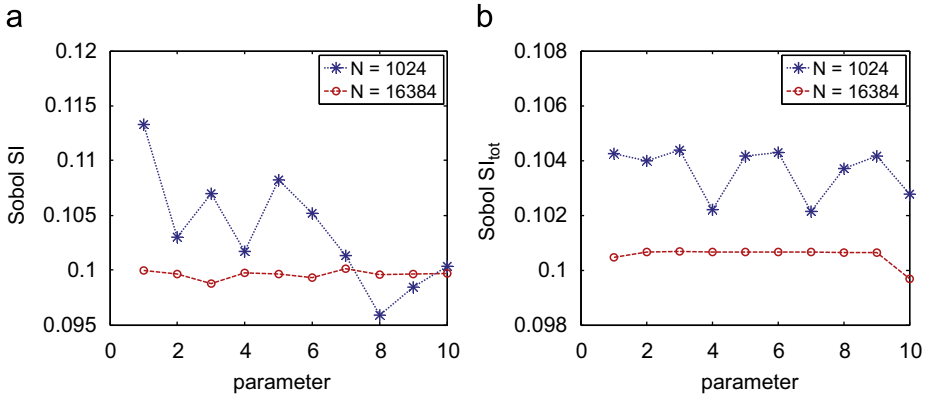

Fig. 7. Numerical evaluation of sensitivity indices S_i (a) and total sensitivity indices S_i^T (b) for B1 function at two different numbers of sampling points $N=1024$ ($N_F=12{,}288$) and $N=16{,}384$ ($N_F=196{,}608$).

variables y and z: $x=(y,\ z)$. Let $y=(x_1,\ldots,x_m)$, $K=(i_1,\ldots,i_m)$, $1\leqslant i_1<\cdots<i_m\leqslant m$. It follows from (11) and (12) that global sensitivity index for a set y is equal to

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

If there is such a small parameter ε, so that condition

$$S_y\geqslant(1-\varepsilon) \tag{20}$$

is satisfied then $d_T=m$.

Global SA offers a general practical way to predict the efficiency of QMC algorithms. Using the Sobol' method of global sensitivity indices the classification of some important classes of integrable functions was developed in [8]. Functions can be divided into three categories with respect to their dependence on the input variables:

Type A—functions with a few dominant variables;

Type B—functions with important low-order interaction terms;

Type C—functions with important high-order interaction terms.

It was shown in [8] that for high-dimensional type A and B functions QMC integration is much more efficient than MC, while for Type C functions efficiencies QMC and MC integrations are similar. These findings are summarised in Table 1. In Section 7, it is shown that DGSM can also be used for classification of functions similar to the one based on the Sobol' method of global sensitivity indices. Criteria that can be used for classification are presented in Table 2.

7. Results

Results obtained by MC and QMC evaluations of DGSM are compared with the Morris method. DGSM are also compared with the Sobol' sensitivity indices to see the analogy between the two types of measures. Seven different test functions were used for comparison (Table 3). Input variables for all functions are uniformly distributed in H^n with $n=10$ apart from the last function for which $n=4$.

The analytical values for the Sobol' sensitivity indices and DGSM were calculated and compared with numerical results. For all tests we calculated analytically the global sensitivity indices S_i, S_i^T and the ratio S_i/S_i^T. We present plots of S_i and S_i^T for each variable for two values of sampling points $N=1024$ and 16,384 and the results of analytical evaluation of measures $\bar{M}_i^*$, $\bar{\Sigma}_i^*$, $\bar{M}_i^*/\bar{\Sigma}_i^*$ and G_i. For the Morris (incremental ratio) and DGSM methods (with numerically evaluated partial derivatives) we plot measures $\bar{M}_i^*$ and $\bar{\Sigma}_i^*$ for each variable x_i for the same number of function evaluations N_F. For all the test functions the same number of sampled points was used ($N=128$). For the DGSM methods in all calculations we used $\delta=10^{-5}$ and for the Morris method the number of levels was $p=10$.

For each of the test functions we also present the RMSE versus the number of sampled points N for the Morris and DGSM methods. To reduce the scatter in the error estimation the values of RMSE were averaged over $L=50$ independent runs:

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

Here I_i^* can be either $\bar{M}_i^*$ or $\bar{\Sigma}_i^*$, I_0 is the corresponding analytical value of $\bar{M}_i^*$ or $\bar{\Sigma}_i^*$. For the MC method all runs were statistically independent. For QMC integration for each run a different part of the Sobol' sequence was used.

RMSE can be approximated by a trend line: $cN^{-\alpha}$. For MC methods the convergence rate α is typically ~0.5, while for QMC methods α~1.0. Values $(-\alpha)$ are given in brackets on the plots of convergence rates.

Results presented in Table 4 for function A1 show that first-order terms are more important than interaction ones for variables with low-order indices: $S_i/S_i^T\geqslant 0.68$ for $i=1,2$, $S_i/S_i^T=0.49$ for $i=3$ but for variables with higher-order indices

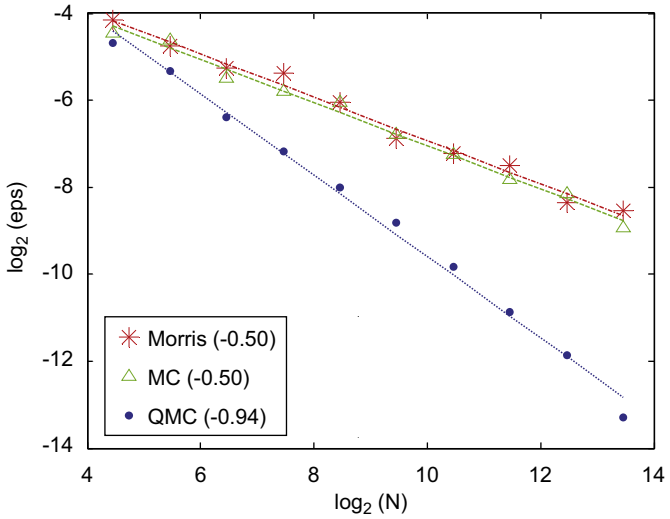

Fig. 9. The integration error of $\bar{M}_i^*$ evaluated by the Morris method and DGSM methods with MC and QMC integrations vs the number of sampled points N. B1 function.

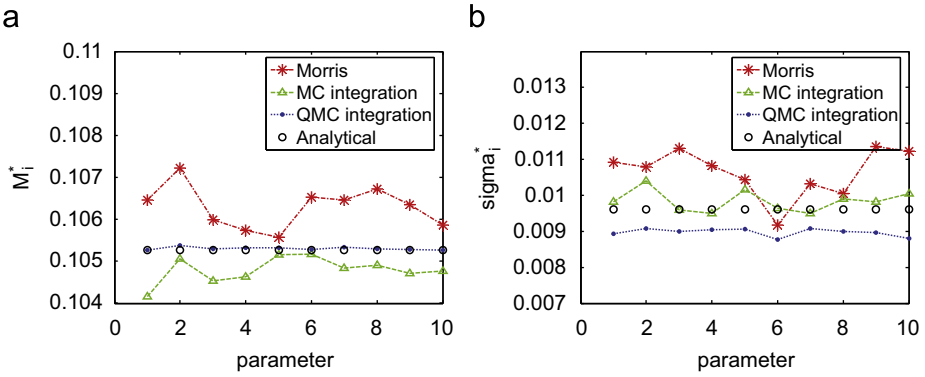

Fig. 8. Comparison of numerical evaluation of $\bar{M}_i^*$ (a) and $\bar{\Sigma}_i^*$ (b) with analytical values for B1 function by the Morris method and DGSM methods with MC and QMC integrations at number of function evaluations $N_F=1408$.

$(i>3)$ $S_i/S_i^T \leqslant 0.36$. It means that high-order interactions are important and $d_S \approx n$. Condition $S_y^T/n_y \gg S_z^T/n_z$ is satisfied for sets $y=\{1,2\}$, $z=\{3,\ldots,10\}$. It confirms that this function is indeed type A function. $S_y=0.89$, hence $d_T=2$ assuming in (20) $\varepsilon \approx 0.1$. For slightly larger set $y=\{1, 2, 3\}$ $S_y=0.96$.

Values of Sobol' indices at $N=1024$ and 16,384 are hardly distinguishable (Fig. 1). Comparison of DGSM obtained with MC and QMC integration with the Morris method at $N_F=1408$ shows that values of $\bar{M}_i^*$ are accurately evaluated by all three methods, however, only QMC integration provides accurate results for $\bar{\Sigma}_i^*$, while the Morris method gives rather inaccurate results for variables x_1 and x_2.

Comparisons of Figs. 1 and 2 show that the general trend of distributions for the Sobol' and DGSM methods are similar. It confirms the assumption of similarity between variance and derivative-based measures. It is easy to see from the last column of table Table 5 (values of G_i) that $d_T \approx 2$.

Fig. 3 shows that for type A functions QMC integration with $\alpha \approx 0.95$ (for $\bar{M}_i^*$) and $\alpha \approx 0.95$ (for $\bar{\Sigma}_i^*$) is much more efficient than MC integration $\alpha \approx 0.51$ (for $\bar{M}_i^*$) and $\alpha \approx 0.51$ (for $\bar{\Sigma}_i^*$). The Morris method has efficiency comparable to that of MC integration.

It was assumed in the past that $\bar{M}_i^*$ is a good proxy for S_i^T [1,10]. However, comparison of ratios $\bar{M}_i^*/S_i^T$ and G_i/S_t^T presented in Table 6 clearly show that only G_i has a direct link with S_i^T ($G_i=\beta S_i^T$, where $\beta=0.89$), while $\bar{M}_i^*$ does not have a simple relationship with S_i^T. Our results confirm an earlier conjecture by Sobol' and Gresham that $S_i \leqslant G_i \leqslant S_i^T$ [9], although their results were concerning only a class of multiplicative functions $f(x)=\prod_{i=1}^{n}\varphi(x_i)$. Table 6 also shows that ratios $\bar{M}_i^*/\bar{\Sigma}_i^*$ are a good proxy to S_i/S_i^T, therefore it can be used for assessing the importance of higher-order interactions in the same way as S_i/S_i^T.

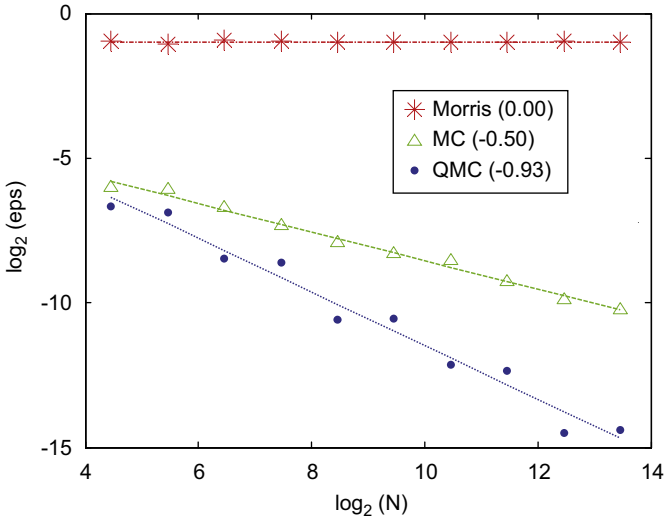

Fig. 12. The integration error of $\bar{M}_1^*$ evaluated by the Morris method and DGSM methods with MC and QMC integrations vs the number of sampled points N. B2 function.

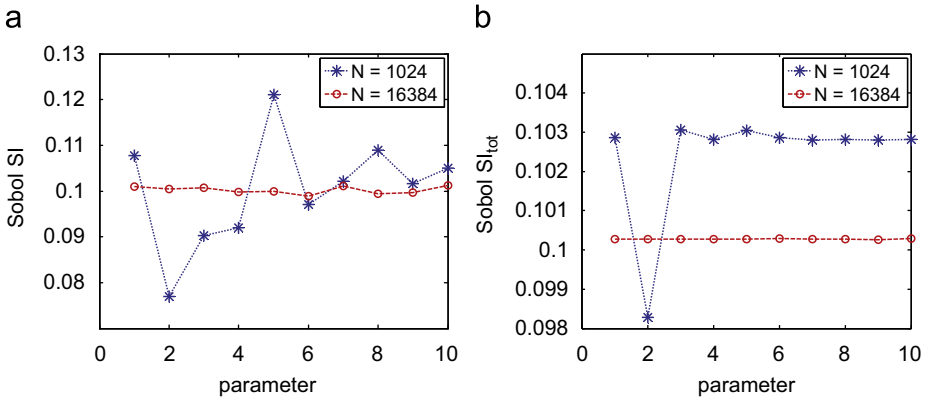

Fig. 10. Numerical evaluation of sensitivity indices S_i (a) and total sensitivity indices S_i^T (b) for B2 function at two different numbers of sampling points $N=1024$ ($N_F=12{,}288$) and $N=16{,}384$ ($N_F=196{,}608$).

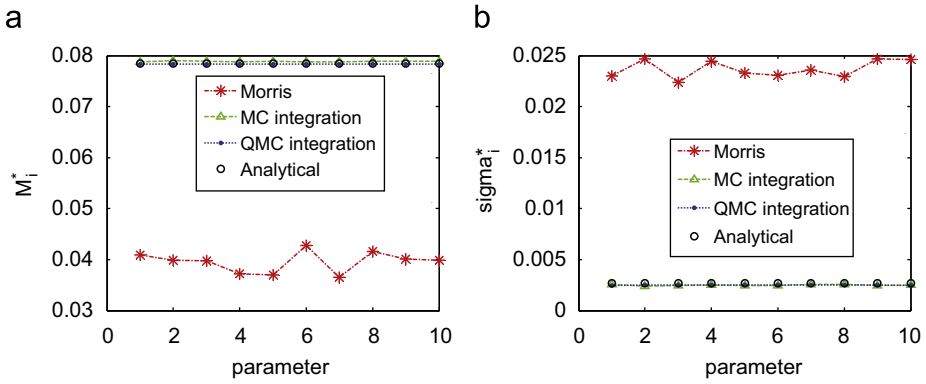

Fig. 11. Comparison of numerical evaluation of $\bar{M}_i^*$ (a) and $\bar{\Sigma}_i^*$ (b) with analytical values for B2 function by the Morris method and DGSM methods with MC and QMC integrations at number of function evaluations $N_F=1408$.

Function A2 is widely used in papers on global SA. It is also known as the "g-function" [1,3]. It can be easily verified that as the value of parameter a_i increases, the importance of the corresponding variable x_i decreases. By varying values of a_i it is possible to change the type of the g-function. For three different sets of $\{a_i\}$ we engineered g-functions of type A (function A2), B (function B2) and C (function C2).

For the g-function analytical values for $\bar{M}_i^*$ and $\bar{\Sigma}_i^*$ are equal to

$$\bar{M}_i^* = \frac{4}{1+a_i},$$

$$\bar{\Sigma}_i^* = \bar{M}_i^* \left[\prod_{k=1,k\neq i}^{n} (1+D_k) - 1 \right]^{1/2}.$$

Here $D_i = 1/(3(1+a_i)^2)$ are partial variances. Analytical values for S_i and S_i^T are given by

$$S_i = \frac{D_i}{D},$$

$$S_i^T = \frac{D_i}{D} \left[\prod_{k=1,k\neq i}^{n} (1+D_k) - 1 \right].$$

Here D is the total variance: $D = \prod_{k=1}^{n}(1+D_k)-1$.

As it follows from Table 7 for function A2 first-order terms are more important than interaction ones ($S_i/S_i^T < 0.5$). It means that $d_S \approx 1$. Condition $S_y^T/n_y \gg S_z^T/n_z$ is satisfied for sets $y = \{1,2\}$, $z = \{3,\ldots,10\}$, therefore $d_T = 2$. A similar result can be obtained from the analysis of Table 8 from which it clearly follows that $d_T = 2$: $\sum_{i=1}^{2} G_i/2 \gg \sum_{i=3}^{n} G_i/8$.

Values of Sobol' indices at $N = 1024$ are not as accurate as the ones at $N = 16{,}384$ especially for S_1 (Fig. 4). A comparison of DGSM obtained with MC and QMC integration with the Morris method at $N_F = 1408$ shows that values of $\bar{M}_i^*$ and $\bar{\Sigma}_i^*$ are accurately evaluated only by MC and QMC integration methods but not by the Morris method (Fig. 5).

From Fig. 6 it follows that QMC integration provides very fast convergence with $\alpha \approx 0.86$ (for $\bar{M}_i^*$) and $\alpha \approx 0.81$ (for $\bar{\Sigma}_i^*$), while for MC integration convergence is much slower with $\alpha \approx 0.51$ (for $\bar{M}_i^*$) and $\alpha \approx 0.52$ (for $\bar{\Sigma}_i^*$). It is important to notice that values for the Morris method do not converge at all with the increase of N.

The g-function is symmetrical with respect to point $x = 0.5$ and it is not differentiable at $x = 0.5$. Evaluation of $E_i(x^*)$ using formula (16) gives a value $E_i(x^*) = -4/(1+a_i)$, $0 \leqslant x^* < 0.5$ and $E_i(x^*) = 4/(1+a_i)$, $0.5 < x^* \leqslant 1.0$. It results in correct values of $\bar{M}_i^*$ and $\bar{\Sigma}_i^*$ when MC or QMC integration of integrals (7) and (8) are used. The situation is different for the Morris method because of the finite value of the increment Δ in (17), evaluation of the elementary effect $EE_i(x^*)$ can give a biased estimate of $E_i(x^*)$: points x_i^* and $x_i^* + \Delta$ can be situated on the opposite sides of the V-shaped g-function slopes ($x_i^* < 0.5$ and $(x_i^* + \Delta) > 0.5$). The situation does not improve much with the increase of the number of levels p. This effect can occur for any non-monotonic function with a characteristic radius of an area of a rapid function change smaller than Δ.

A comparison of ratios $\bar{M}_i^*/S_i^T$ and G_i/S_i^T presented in Table 9 unequivocally shows that $G_i = \beta S_i^T$, where $\beta = 0.9$, while there is no such a link between $\bar{M}_i^*$ and S_i^T. It also follows from Table 9 that there is a link between $\bar{M}_i^*/\bar{\Sigma}_i^*$ and S_i/S_i^T.

Table 14
Analytical values for indices S_i, S_i^T and the ratio S_i/S_i^T for function C1

x_i	S_i	S_i^T	S_i/S_i^T
$i = 1$–10	2.0×10^{-2}	0.27	7.5×10^{-2}

Table 15
Analytical values for $\bar{M}_i^*$, $\bar{\Sigma}_i^*$, $\bar{M}_i^*/\bar{\Sigma}_i^*$, $\sqrt{\bar{M}_i^{*2} + \bar{\Sigma}_i^{*2}}$ and G_i for function C1

x_i	$\bar{M}_i^*$	$\bar{\Sigma}_i^*$	$\bar{M}_i^*/\bar{\Sigma}_i^*$	$\sqrt{\bar{M}_i^{*2} + \bar{\Sigma}_i^{*2}}$	G_i
$i = 1$–10	2.0	7.02	0.28	7.30	0.1

Table 16
Analytical values for indices S_i, S_i^T and the ratio S_i/S_i^T for function C2

x_i	S_i	S_i^T	S_i/S_i^T
$i = 1$–10	2.0×10^{-2}	0.27	7.5×10^{-2}

Table 17
Analytical values for $\bar{M}_i^*$, $\bar{\Sigma}_i^*$, $\bar{M}_i^*/\bar{\Sigma}_i^*$, $\sqrt{\bar{M}_i^{*2} + \bar{\Sigma}_i^{*2}}$ and G_i for function C2

x_i	$\bar{M}_i^*$	$\bar{\Sigma}_i^*$	$\bar{M}_i^*/\bar{\Sigma}_i^*$	$\sqrt{\bar{M}_i^{*2} + \bar{\Sigma}_i^{*2}}$	G_i
$i = 1$–10	4.0	14.04	0.28	14.6	0.1

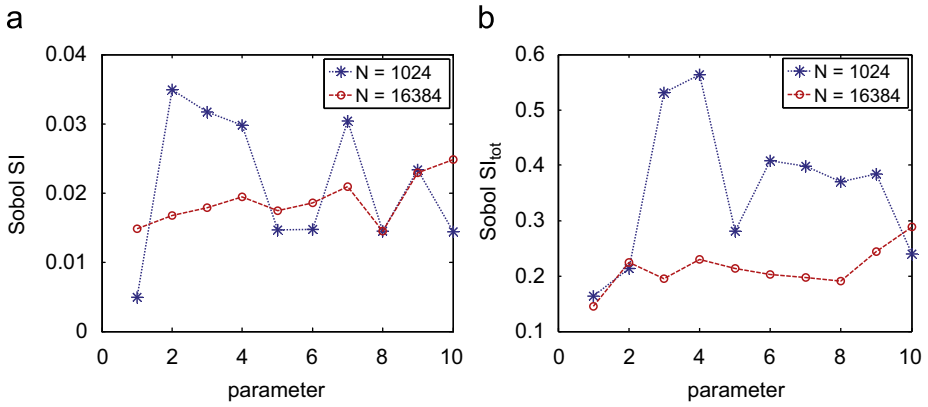

Fig. 13. Numerical evaluation of sensitivity indices S_i (a) and total sensitivity indices S_i^T (b) for C1 function at two different numbers of sampling points $N = 1024$ ($N_F = 12{,}288$) and $N = 16{,}384$ ($N_F = 196{,}608$).

Type B functions B1 and B2 have the same values of S_i and S_i^T ($S_i = S_i^T = 1/n$) due to the dominance of main effects (Tables 10 and 12). Values of $d_T = 10$ and $d_S = 1$ are also the same for both functions. In comparison with Type A functions evaluation of global sensitivity indices becomes slightly less efficient as Figs. 7 and 10 show: at $N = 1024$ the values of S_i and S_i^T are evaluated with the relative error approximately equal to 20% (S_i) and 5% (S_i^T).

For functions B1 and B2 the ratio $\bar{M}_i^*/\bar{\Sigma}_i^* > 1$ (Tables 11 and 13), which means that higher-order interactions are negligible. This conclusion is consistent with the condition $S_i/S_i^T \approx 1$ (Tables 12 and 13).

A comparison of values $\bar{M}_i^*$ and $\bar{\Sigma}_i^*$ in Figs. 8 and 11 show that the QMC integration method is the most accurate in evaluating DGSM while the Morris method is the least accurate among the three methods. Figs. 9 and 12 confirm that the integration errors for both type B functions exhibit a similar behaviour with QMC outperforming MC by several orders of magnitude. For function B1 the Morris method and the DGSM with MC integration method show a similar convergence. For function B2 the Morris method converges to a value, which is roughly two times larger than analytical value for $\bar{M}_i^*$ and 8 times larger than analytical value for $\bar{\Sigma}_i^*$ due to the reason explained above. The accuracy of the Morris method does not improve with the increase of N (Figs. 10–12).

Type C functions C1 and C2 have the same values of S_i and S_i^T (Tables 14 and 16). For these functions $S_i/S_i^T \ll 1$, higher-order interactions play a dominant role; d_T and d_S are both equal to $n = 10$. Values of the ratio $\bar{M}_i^*/\bar{\Sigma}_i^*$ are less than 1, which confirms that high-order interactions are important (Tables 15 and 17).

For this type of function QMC integration can lose its advantage over MC. To achieve good accurate evaluation of Sobol' sensitivity indices, a high number of sampled points is required. Figs. 13 and 16 show that even at rather high value of $N = 16{,}384$ ($N_F = 196{,}608$) values of S_i and S_i^T are evaluated with the relative error approximately equal to 10% (Tables 16 and 17).

For functions C1 and C2, QMC and MC methods produce reasonably accurate results for DGSM at $N_F = 1408$ (Figs. 14 and 17). The Morris method is the least accurate method among the three methods. It also exhibits highly oscillating behaviour of evaluated $\bar{M}_i^*$ and $\bar{\Sigma}_i^*$ values.

Fig. 15 shows that the convergence rates of all three methods for function C1 are similar, although the QMC method still outperforms other two methods. The situation is different for function C2: the QMC and MC methods show similar performance with the QMC method being marginally more efficient; however, the convergence curve for the Morris only originally decreases with N but at higher values of N it reaches a constant value, which is not shown in Fig. 18 due to the limited number of sample points $N = 2^{14}$ used for presentation. It is explained by the fact that for function C2 the evaluated values of $\bar{M}_i^*$ and $\bar{\Sigma}_i^*$ do not converge to the true analytical values of DGSM.

Function A3 was used in papers on the Morris method [16]. It is clear from Table 18 that the first two variables are more important than variables 3 and 4. The same results can be seen from Table 19. The ratio G_i/S_i^T is close to a constant, which shows that these two measures provide very similar information about importance of variables (Table 19). The ratio $(\bar{M}_i^*/\bar{\Sigma}_i^*)/(S_i/S_i^T)$ is also reasonably constant (within 30% accuracy). It proves that the ratio $\bar{M}_i^*/\bar{\Sigma}_i^*$ can be used for analysis of the importance of higher-order terms (Figs. 16–18).

Table 18
Analytical values for indices S_i, S_i^T and the ratio S_i/S_i^T for function A3

x_i	S_i	S_i^T	S_i/S_i^T
1	0.38	0.43	0.89
2	0.37	0.41	0.90
3	7.9×10^{-2}	9.3×10^{-2}	0.85
4	0.11	0.13	0.85

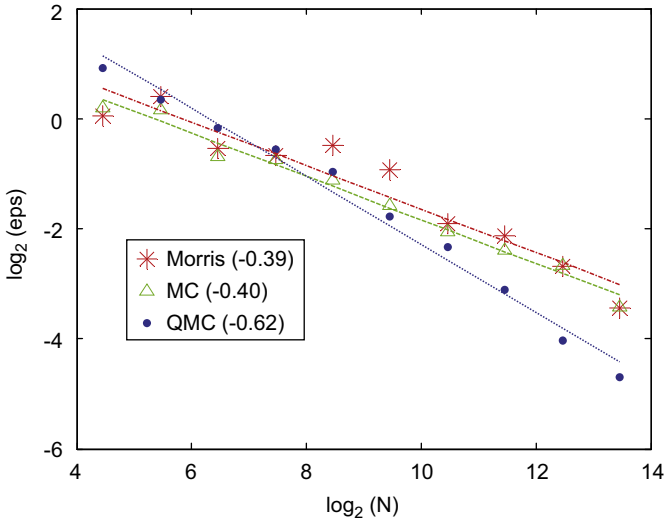

Fig. 15. The integration error of $\bar{M}_1^*$ evaluated by the Morris method and DGSM methods with MC and QMC integrations vs the number of sampled points N. C1 function.

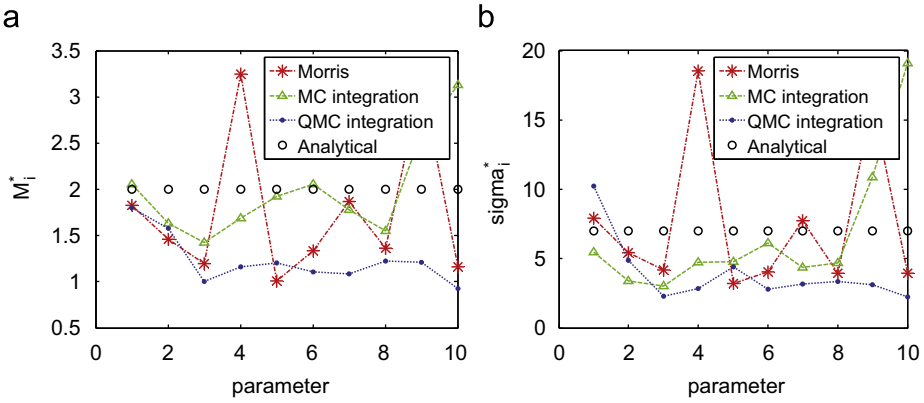

Fig. 14. Comparison of numerical evaluation of $\bar{M}_i^*$ (a) and $\bar{\Sigma}_i^*$ (b) with analytical values for C1 function by the Morris method and DGSM methods with MC and QMC integrations at number of function evaluations $N_F = 1408$.

Function A3 is low-dimensional ($n = 4$), hence all methods show reasonably good values of numerical estimation of Sobol' sensitivity indices and DGSM measures (Figs. 19 and 20). However, Fig. 21 shows that the QMC method is much more efficient in terms of the convergence rate than the MC and the Morris methods (Table 20).

Table 21 presents computational costs for DGSM and the Morris methods at 1% accuracy of evaluated values of $\tilde{M}_1^*$. It follows from the table that the MC-based DGSM method is approximately 2 times more efficient than the Morris method for the considered type A functions and it is almost 10 times more efficient for the type C functions. For the function B1 the Morris and the MC-based DGSM methods showed a similar performance.

The QMC-based DGSM method is approximately 38 times more efficient in terms of the CPU time and 8 times more efficient in terms of the number of sampled points than the Morris method for the C1 function. It is also much more efficient than the Morris method for the type A and B functions. For the type B function the ratio of efficiency of QMC to MC-based methods is approximately equal to 4 and it drops to 2 (number of sampled points) and 3 (CPU time) for the type C functions.

Table 19

Analytical values for $\tilde{M}_i^*$, $\tilde{\Sigma}_i^*$, $\tilde{M}_i^*/\tilde{\Sigma}_i^*$, $\sqrt{\tilde{M}_i^{*2}+\tilde{\Sigma}_i^{*2}}$ and G_i for function A3

x_i	$\tilde{M}_i^*$	$\tilde{\Sigma}_i^*$	$\tilde{M}_i^*/\tilde{\Sigma}_i^*$	$\sqrt{\tilde{M}_i^{*2}+\tilde{\Sigma}_i^{*2}}$	G_i
1	92.85	32.89	2.82	98.51	0.39
2	90.34	39.71	2.27	98.68	0.39
3	42.17	16.84	2.50	45.41	0.08
4	49.28	26.82	1.83	56.11	0.32

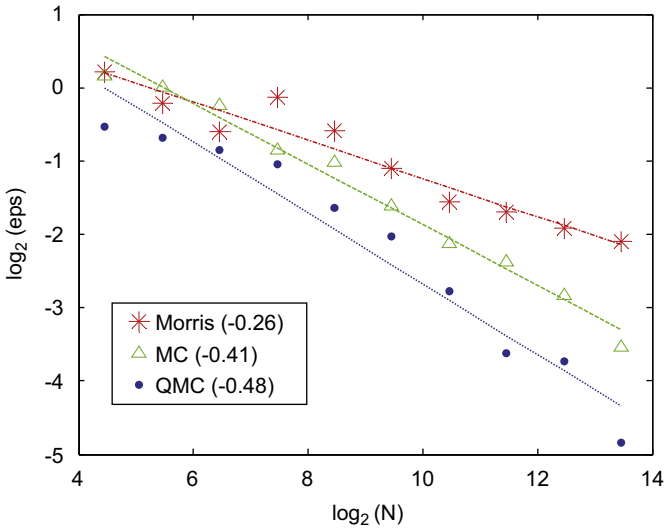

Fig. 18. The integration error of $\tilde{M}_1^*$ evaluated by the Morris method and DGSM methods with MC and QMC integrations vs the number of sampled points N. C2 function.

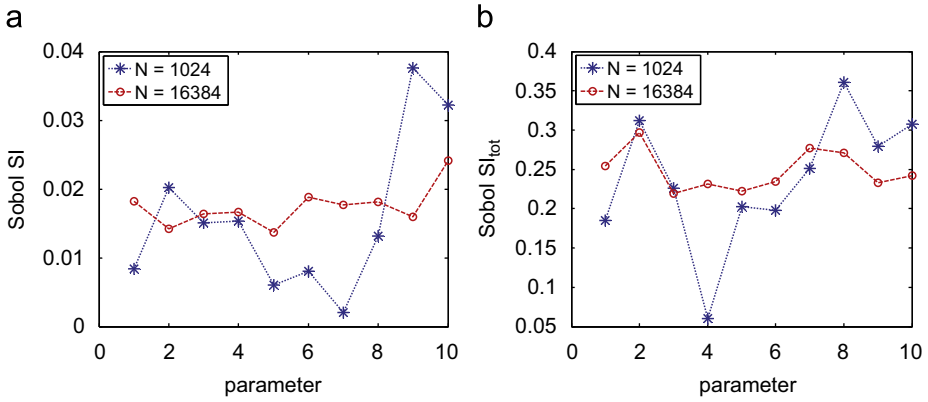

Fig. 16. Numerical evaluation of sensitivity indices S_i (a) and total sensitivity indices S_i^T (b) for C2 function at two different numbers of sampling points $N = 1024$ ($N_F = 12{,}288$) and $N = 16{,}384$ ($N_F = 196{,}608$).

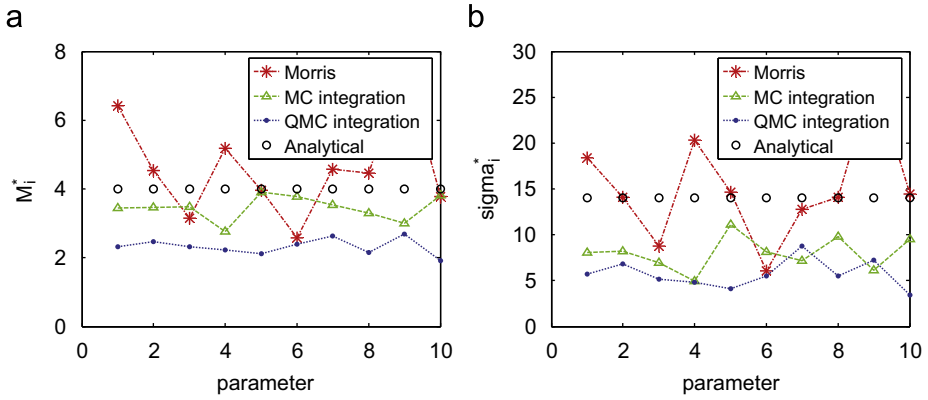

Fig. 17. Comparison of numerical evaluation of $\tilde{M}_i^*$ (a) and $\tilde{\Sigma}_i^*$ (b) with analytical values for C2 function by the Morris method and DGSM methods with MC and QMC integrations at number of function evaluations $N_F = 1408$.

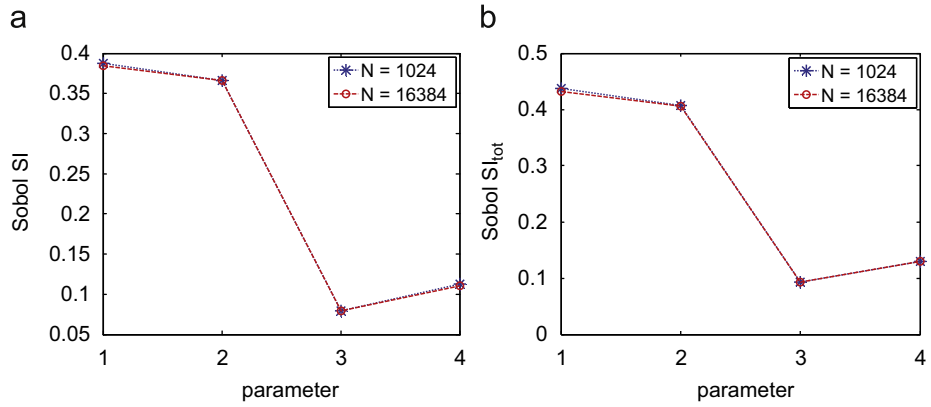

Fig. 19. Numerical evaluation of sensitivity indices S_i (a) and total sensitivity indices S_i^T (b) for A3 function at two different numbers of sampling points $N = 1024$ ($N_F = 6144$) and $N = 16{,}384$ ($N_F = 98{,}304$).

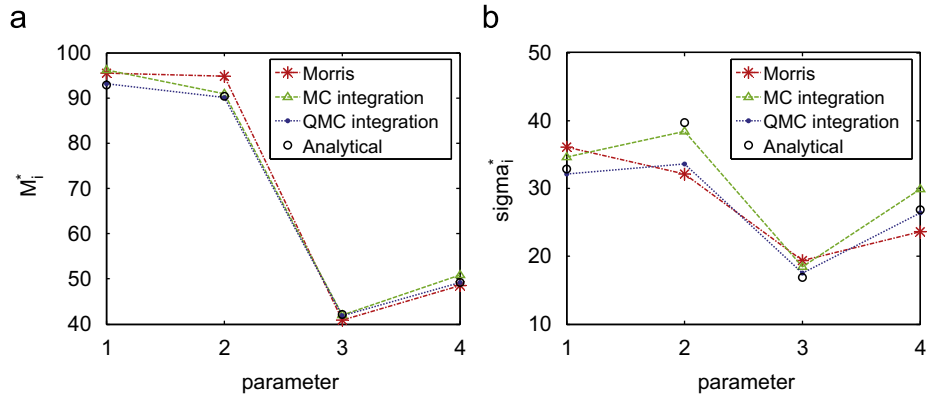

Fig. 20. Comparison of numerical evaluation of $\bar{M}_i^*$ (a) and $\bar{\Sigma}_i^*$ (b) by the Morris method and DGSM methods with MC and QMC integrations with analytical values for A3 function at number of function evaluations $N_F = 640$.

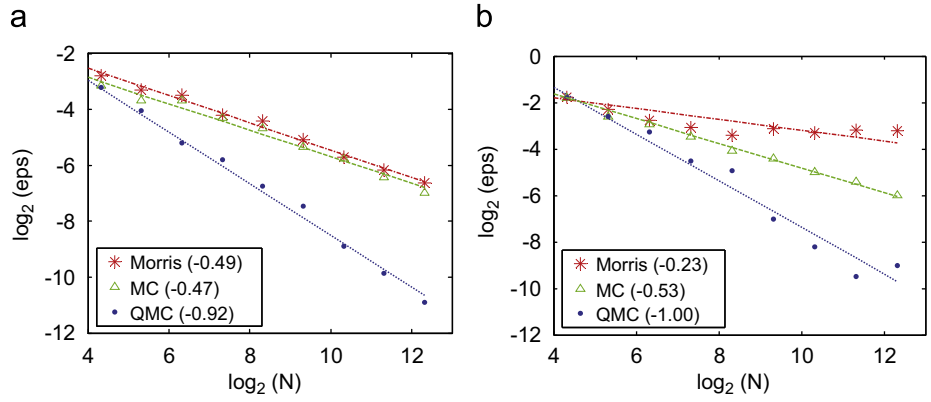

Fig. 21. The integration error of $\bar{M}_1^*$ (a) and $\bar{\Sigma}_1^*$ (b) evaluated by the Morris method and DGSM methods with MC and QMC integrations vs the number of sampled points N. A3 function.

Table 20
Ratios G_i/S_i^T and $(\bar{M}_i^*/\bar{\Sigma}_i^*)/(S_i/S_i^T)$ for function A3

x_i	G_i/S_i^T	$(\bar{M}_i^*/\bar{\Sigma}_i^*)/(S_i/S_i^T)$
1	0.92	3.17
2	0.96	2.52
3	0.90	2.94
4	0.98	2.15

As shown in [10], the efficiency of the Morris method can be significantly improved by applying optimised sampling strategy. We also note that the Morris method is traditionally used as a screening method at a very low number of sampled points. Although at such a number of points the values of the Morris measures can be very far from the converged ones, the high accuracy of estimates may not be required for screening purposes.

Table 21
CPU time and number of sampled points required for achieving 1% accuracy of evaluated values of $\widetilde{M}_1^*$ for the Morris method and for the DGSM methods based on MC and QMC samplings

Function	Morris		DGSM (MC)		DGSM (QMC)	
	CPU time	*N*	CPU time	*N*	CPU time	*N*
A1	1.33	11,264	0.55	5632	0.10	704
B1	0.12	704	0.10	704	0.02	88
C1	1398.10	1,441,792	139.06	360,448	36.59	180,224
C2	–	–	439.34	720,869	154.33	360,448

8. Conclusions

In this paper, we have considered derivative-based global sensitivity measures (DGSM). We have presented an efficient and general algorithm for evaluation of the DGSM based on MC and QMC integration methods. It has been proven that this approach can be much faster and more accurate than the Morris method. However, in many instances the Morris method still can be seen as a good compromise between accuracy and efficiency.

Different types of test functions have been used for testing and comparison. For functions with low effective dimensions the QMC method shows much higher convergence rate than the MC or the Morris methods. It has been shown that the Morris method can produce inaccurate measures for non-monotonic functions.

It has been established empirically that there is a link between DGSM and Sobol' global sensitivity indices. The computational time required for numerical evaluation of DGSM measures is many orders of magnitude lower than that for estimation of the Sobol' global sensitivity indices.

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