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The identification of model effective dimensions using global sensitivity analysis

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ABSTRACT

It is shown that the effective dimensions can be estimated at reasonable computational costs using variance based global sensitivity analysis. Namely, the effective dimension in the truncation sense can be found by using the Sobol' sensitivity indices for subsets of variables. The effective dimension in the superposition sense can be estimated by using the first order effects and the total Sobol' sensitivity indices. The classification of some important classes of integrable functions based on their effective dimension is proposed. It is shown that it can be used for the prediction of the QMC efficiency. Results of numerical tests verify the prediction of the developed techniques.

1. Introduction

Modern mathematical models of real systems in physics, chemistry, biology, economics and other areas often have high complexity with hundreds or even thousands of variables. Straightforward modelling using such models can be computationally costly or even impossible. There is a demand for complexity reduction techniques which are not only general and applicable to any complex non-linear model but also rigorous in that their application provides estimates of the approximation errors. Variance based global sensitivity analysis allows to develop such complexity reduction techniques. Recently a new class of measures was introduced by Borgonovo [1,2]. These measures are known as moment-independent. They are based on the entire distribution of the output without a specific reference to its moments. Potentially, moment-independent measures can also be used for complexity reduction.

For modelling and complexity reduction purposes it is important to distinguish between the model nominal dimension and its effective dimension. The notions of the "effective dimension" in the truncation and superposition sense was introduced by Caflisch et al. in [3]. Quite often complex mathematical models have effective dimensions much lower than their nominal dimensions. The knowledge of model effective dimensions is very important as it allows to apply various complexity reduction techniques.

The effective dimension in the truncation sense d_T loosely speaking is equal to the number of important factors in the model. Identification of important and not important variables allows to fix not important variables at their nominal values. The resultant model would have lower complexity with dimensionality reduced from n to d_T. A condition $d_T \ll n$ often occurs in practical problems. Another type of complexity reduction is associated with the effective dimension in the superposition sense d_S: the function has the effective dimension in the superposition sense d_S if it is almost a sum of s-dimensional function components in the ANOVA decomposition.

For some problems such as path-dependent option pricing in mathematical finance changing the order in which input variables are sampled can dramatically decrease d_T. Such techniques are known as dimension reduction. Most results on dimension reduction are empirical and qualitative (see for example [3]).

A straightforward evaluation of the effective dimensions from their definitions is not practical in the general. Owen introduced the dimension distribution for a square integrable function [4]. The effective dimension can be defined through a quantile of the dimension distribution. He showed that for some classes of functions quantiles of the dimension distribution can be explicitly calculated but they are difficult to estimate in a general case. In this paper we show that global sensitivity analysis based on the Sobol' sensitivity indices (SI) allows to estimate the effective dimensions at reasonable computational costs.

Evaluation of the Sobol' SI necessitates the computation of high-dimensional integrals. The classical grid methods become computationally impractical when the number of dimensions n increases

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because of "the curse of dimensionality". The convergence rate of Monte Carlo (MC) integration methods does not depend on the number of dimensions n. However, the rate of convergence $O(N^{-1/2})$, where N is the number of sampled points, attained by MC is rather slow. A higher rate of convergence can be obtained by using quasi-Monte Carlo (QMC) methods based on uniformly distributed sequences instead of pseudo-random numbers. Asymptotically, QMC can provide the rate of convergence $O(N^{-1})$.

For sufficiently large N, QMC should always outperform MC. However, in practice such sample sizes quite often are infeasible, especially when high-dimensional problems are concerned. Many numerical experiments demonstrated that the advantages of QMC can disappear for high-dimensional problems. There were claims that the degradation in performance of QMC occurs at $n \geq 12$ [5]. In contrast, other papers reported the superiority of QMC over MC for some integrands with $n = 360$ [6]. Some explanations for such inconsistent results were given using the notion of the effective dimension [3]. In [7] it was shown how the ANOVA components are linked to the effectiveness of QMC integration methods. Sloan and Wozniakowski [8] studied the efficiency of the quasi-Monte Carlo algorithms for high-dimensional integrals. They identified classes of functions for which the effect of the dimension is negligible. These are the so-called weighted classes in which the behavior in the successive dimensions is moderated by a sequence of weights.

There is no computationally feasible technique that would predict the efficiency of QMC in high dimensions. In this paper we use Sobol' SI as a quantitative measure of the QMC efficiency.

This paper is organized as follows. Section 2 briefly describes MC and QMC integration algorithms and issues concerning the possible degradation of QMC efficiency in higher dimensions. Section 3 gives a description of the Sobol' SI. Section 4 presents improved formulas for evaluation of the Sobol' SI. The notion of the effective dimension is introduced in Section 5. The classification of functions based on Sobol' SI is suggested in Section 6. It is shown how this classification can be used for the prediction of the QMC efficiency. Test examples and numerical results are considered in Section 7. Finally, conclusions are given in Section 8.

2. MC and QMC algorithms

Consider the evaluation of an integral

$$I[f] = \int_{H^n} f(\mathbf{x})\, d\mathbf{x},$$

where the function $f(\mathbf{x})$ is integrable in the n-dimensional unit hypercube H^n and sufficiently regular. The Monte Carlo quadrature formula is based on the probabilistic interpretation of an integral. An approximation to this expectation is

$$I_N[f] \approx \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i),$$

where $\{\mathbf{x}_i\}$ 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 ε defined as

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

The expectation of ε^2 is

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

where $\sigma^2(f)$ is the variance. The root mean square error of the MC method is

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

In contrast to grid methods, the convergence rate of MC methods does not depend on the number of variables n although it is rather slow.

The efficiency of MC methods is determined by the properties of the random numbers. Random number sampling is prone to clustering. As new points are added randomly, they do not necessarily fill the gaps between already sampled points. In contrast, low-discrepancy sequences (LDS) are specifically designed to place sample points as uniformly as possible.

The discrepancy is the measure of deviation from uniformity. Consider a number of points N from a sequence $\{\mathbf{x}_i\}$ in an n-dimensional rectangle Q whose sides are parallel to the coordinate axes, $Q \in H^n$. Then, the discrepancy is defined as

$$D_N = \sup_{Q \in H^n} \left| \frac{N_Q}{N} - m(Q) \right|,$$

where $m(Q)$ is a volume of Q and N_Q is the number of points of the sequence $\{x_i\}$ that are contained in Q.

The Koksma–Hlawka inequality gives an upper bound for the QMC integration error:

$$\varepsilon_{QMC} \leq V(f) D_N. \tag{1}$$

Here, $V(f)$ is the variation of $f(\mathbf{x})$ in the sense of Hardy and Krause [9]. For a one-dimensional function with a continuous first derivative it is simply

$$V(f) = \int_{H^1} |df(x)/dx|\, dx. \tag{2}$$

In higher dimensions, the Hardy-Krause variation may be defined in terms of the integral of partial derivatives. Further it is assumed that $f(\mathbf{x})$ is a function of bounded variation.

For random numbers, the expected discrepancy is $D_N = O((\ln\ln N)/N^{1/2})$, while the discrepancy of LDS is of the order

$$D_N = O\left(\frac{\log^n(N)}{N}\right). \tag{3}$$

There are a few well-known and commonly used LDSs. Different principles were used for their construction by Halton, Faure, Sobol, Niederreiter and others. The LDS developed by Niederreiter has the best theoretical asymptotic properties [9]. However, many practical studies have proven that the Sobol' LDS is in many aspects superior to other LDS [6,10].

The Sobol' LDS was constructed by following the three main requirements [11]:

1. Best uniformity of distribution as $N \to \infty$.
2. Good distribution for fairly small initial sets.
3. A very fast computational algorithm.

Points generated by the Sobol' LDS produce a very uniform filling of the space even for a rather small number of points N, which is a very important point in practice.

The bound on the integration error (1) is a weak one and is not particularly meaningful in practice. It was shown experimentally that the QMC integration error is determined by the variance and not by the variation of the integrand [12]. It is generally accepted that the rate of the discrepancy determines the expected rate of the accuracy, so one can use an estimate of the QMC convergence rate

$$\varepsilon_{QMC} = O\left(\frac{\log^n(N)}{N}\right). \tag{4}$$

Asymptotically, this rate of convergence is $O(N^{-1})$. Numerous computational studies showed that QMC methods can provide significant improvement over MC. The analysis of (4) shows that ε_{QMC} is an increasing function of N up to some threshold value of N^*, $N^* \approx \exp(n)$. The accelerated convergence rate $O(N^{-1})$ sets in at

$N > N^*$. For high-dimensional problems such a large number of sample points is infeasible. This is one of the reasons why in practice the advantages of using QMC can disappear at high and even moderate values of n.

The study of some test problems in [5] led its authors conclude that even for problems of moderate dimensionality ($n > 12$) QMC offers no practical advantage over MC. Other authors [13,14] also reported the degradation of performance of QMC in high dimensions and for a discontinuous function even in low dimensions. In contrast, in [6] it was found that for some high-dimensional integrands ($n = 360$), QMC significantly outperformed MC. These results were later confirmed in other papers (e.g. [3,4,15]).

Sobol noted that an error bound (1) with D_N given by (3) was obtained with the assumption that the function $f(\mathbf{x})$ depends equally on all variables [16]. In practical applications many functions quite often strongly depend only on a small subset of variables: $x_{i_1}, x_{i_2}, \ldots, x_{i_s}, 1 \le i_1 < i_2 < \cdots < i_s, s < n$ while the dependence on other variables can be weak. In this case, n can be substituted by s in (4). This consideration is based on a very important property of LDS: the projection of the n-dimensional LDS on the s-dimensional subspace forms the s-dimensional LDS. That means in particular that the accelerated convergence rate of the QMC integration can set in at lower values of $N > N^*, N^* \approx \exp(s)$. It is important to note that in practice low-dimensional projections have good uniform distributions, while in high dimensions LDS are not particularly well equidistributed for feasible N.

The effects on the convergence of certain properties of integrands including variance, variation, smoothness and dimension were studied in [14]. It was found that the variation does not affect the convergence, while the variance provides a rough upper bound, but it does not accurately predict the performance.

Caflisch et al. [3] introduced the notion of an effective dimension. It was suggested that QMC is superior to MC if the effective dimension of an integrand is not too large. The notion is based on the ANalysis Of VAriances (ANOVA). In [7] it was shown how the ANOVA components are linked to the effectiveness of QMC integration methods. Owen [4] introduced the dimension distribution for square integrable functions and showed how it is linked with Sobol' SI [17] . Further details are given in Section 5.

3. Global sensitivity indices

Many practical problems deal with functions of a very complex structure. Global sensitivity analysis (SA) can provide information on the general structure of a function by quantifying the variation in the output variables to the variation of the input variables. The method of global SA is superior to the local SA methods such as regression analysis, rank transformation, etc. as it is general and can be applied to both linear and highly non-linear functions [18]. One of the most efficient global SA techniques is based on the Sobol' SI [17]. This technique provides an unambiguous information on the importance of different subsets of input variables to the output variance.

Consider an integrable function $f(\mathbf{x})$ defined in the unit hypercube H^n. It can be expanded in the following form:

$$f(\mathbf{x}) = f_0 + \sum_{s=1}^{n} \sum_{i_1 < \cdots < i_s}^{s} f_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s}). \tag{5}$$

This expansion is a sum of 2^n components. It can also be presented as

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{i<j}^{n} f_{ij}(x_i, x_j) + \cdots + f_{12\ldots n}(x_1, x_2, \ldots, x_n).$$

Each of the components $f_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s})$ is a function of a unique subset of variables from $\mathbf{x}$. The components $f_i(x_i)$ are called first order terms, $f_{ij}(x_i, x_j)$ the second order terms and so on.

It can be proven [17] that the expansion (5) is unique if

$$\int_{H^n} f_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s})\, dx_{i_k} = 0, \quad 1 \le k \le s, \tag{6}$$

in which case it is called a decomposition into summands of different dimensions [19]. This decomposition was introduced in [20,19]. Later it became known as the ANOVA decomposition. The ANOVA decomposition is orthogonal, i.e. for any two subsets $\mathbf{u} \ne \mathbf{w}$ an inner product

$$\int_{H^n} f_{\mathbf{u}}(\mathbf{x}) f_{\mathbf{w}}(\mathbf{x})\, d\mathbf{x} = 0. \tag{7}$$

It follows from (5) and (6) that

$$\int_{H^n} f(\mathbf{x})\, d\mathbf{x} = f_0,$$

$$\int_{H^n} f(\mathbf{x}) \prod_{k \ne i} dx_k = f_0 + f_i(x_i),$$

$$\int_{H^n} f(\mathbf{x}) \prod_{k \ne (i,j)} dx_k = f_0 + f_i(x_i) + f_j(x_j) + f_{i,j}(x_i, x_j) \tag{8}$$

and so on.

For square integrable functions, the variances of the terms in the ANOVA decomposition add up to the total variance of the function

$$\sigma^2 = \sum_{s=1}^{n} \sum_{i_1 < \cdots < i_s}^{n} \sigma^2_{i_1 \ldots i_s}, \tag{9}$$

where $\sigma^2_{i_1 \ldots i_s} = \int_{H^n} f^2_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s})\, dx_{i_1} \ldots dx_{i_s}$.

Sobol' defined the global SI as the ratios

$$S_{i_1 \ldots i_s} = \frac{\sigma^2_{i_1 \ldots i_s}}{\sigma^2}.$$

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

$$\sum_{s=1}^{n} \sum_{i_1 < \cdots < i_s}^{n} S_{i_1 \ldots i_s} = 1.$$

$S_{i_1 \ldots i_s}$ can be viewed as a natural sensitivity measure of a set of variables $x_{i_1}, \ldots, x_{i_s}$. It corresponds to a fraction of the total variance given by $f_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s})$. For example, S_1 is the main effect of a variable x_1, S_{12} is a measure of interactions between x_1 and x_2 (i.e. that part of the total variance due to parameters x_1 and x_2 which cannot be explained by the sum of the effects of parameters x_1 any x_2) and so on. For functions of an additive structure, only the low-order SI are important. In an extreme case in which there is no interaction among the input variables,

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^{n} f(x_i)$$

all higher order SI are equal to zero. Thus,

$$\sum_{i=1}^{n} S_i = 1.$$

This case is very important for the understanding of the performance of QMC integration. It will be considered in the following section.

In the general case, all SI can be important for SA. Their straightforward calculation using the ANOVA decomposition would result in 2^n integral evaluations of the summands $f_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s})$ using (8) and 2^n integral evaluations for calculations of $\sigma^2_{i_1 \ldots i_s}$ (9). For high-dimensional problems such an approach is impractical. For this reason Sobol' introduced the SI for subsets of variables. Consider two complementary subsets of variables $\mathbf{y}$ and $\mathbf{z}$:

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

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

$$\sigma_y^2=\sum_{s=1}^{m}\sum_{(i_1<\cdots<i_s)\in K}\sigma^2_{i_1,\ldots,i_s}.$$

σ_y^2 includes all partial variances $\sigma^2_{i_1},\sigma^2_{i_2},\ldots,\sigma^2_{i_1\ldots i_s}$ such that their subsets of indices $(i_1,\ldots,i_s)\in K$. The variance σ_z^2 is defined similarly. The total variance $(\sigma_y^{tot})^2$ is defined as

$$(\sigma_y^{tot})^2=\sigma^2-\sigma_z^2.$$

$(\sigma_y^{tot})^2$ consists of all $\sigma^2_{i_1\ldots i_s}$ such that at least one index $(i_p)\in K$ while the remaining indices can belong to the complimentary set $\overline{K}$. The corresponding global SI are defined as

$$S_y=\frac{\sigma_y^2}{\sigma^2},$$

$$S_y^{tot}=\frac{(\sigma_y^{tot})^2}{\sigma^2}.$$

Obviously $S_y^{tot}=1-S_z$. $S_y^{tot}-S_y$ accounts for all interactions between $\mathbf{y}$ and $\mathbf{z}$. The total sensitivity indices were introduced by Homma and Saltelli in [21].

The important indices in practice are S_i and S_i^{tot}. Their knowledge in most cases provides sufficient information to determine the sensitivity of the analyzed function to individual input variables. The use S_i and S_i^{tot} reduces the number of index calculations from $O(2^n)$ to just $O(2n)$. Extreme cases are

- $S_i^{tot}=0$ means that $f(\mathbf{x})$ does not depend on x_i (in this case S_i is also equal to 0);
- $S_i=1$ means that $f(\mathbf{x})$ depends only on x_i (in this case S_i^{tot} is also equal to 1);
- $S_i=S_i^{tot}$ corresponds to the absence of interactions between variable x_i and other variables. It will be shown in the next section how this case relates to the efficiency of QMC integration.

4. Original and improved formulas for evaluation of SI

One of the most important results obtained by Sobol' is an effective way of computing SI. Given $\mathbf{x}$ and $\mathbf{x}'$ being two independent sample points, where $\mathbf{x}=(\mathbf{y},\mathbf{z})$ and $\mathbf{x}'=(\mathbf{y}',\mathbf{z}')$, S_y and S_y^{tot} are calculated using the following formulae [22]:

$$S_y=\frac{\int_0^1 f(\mathbf{x})f(\mathbf{y},\mathbf{z}')\,d\mathbf{x}\,d\mathbf{z}'-f_0^2}{\int_0^1 f^2(\mathbf{x})\,d\mathbf{x}-f_0^2},\tag{10}$$

$$S_y^{tot}=\frac{1}{2}\frac{\int_{H^n}[f(\mathbf{x})-f(\mathbf{y}',\mathbf{z})]^2\,d\mathbf{x}\,d\mathbf{y}'}{\int_0^1 f^2(\mathbf{x})\,d\mathbf{x}-f_0^2}.\tag{11}$$

In the general multidimensional case, the integrals in (10) and (11) are evaluated using MC or QMC methods.

Formulae (10), (11) are based on generating two independent sample points $\mathbf{x}=(\mathbf{y},\mathbf{z})$, $\mathbf{x}'=(\mathbf{y}',\mathbf{z}')$ and evaluating the three functions $f(\mathbf{x}),f(\mathbf{y},\mathbf{z}'),f(\mathbf{y}',\mathbf{z})$. In this case a Monte Carlo algorithm for (10) has a form

$$S_y\approx\frac{\frac{1}{N}\sum_{i=1}^{N}f(\mathbf{y},\mathbf{z})f(\mathbf{y},\mathbf{z}')-\left[\frac{1}{N}\sum_{i=1}^{N}f(\mathbf{y},\mathbf{z})\right]^2}{\frac{1}{N}\sum_{i=1}^{N}f^2(\mathbf{y},\mathbf{z})-\left[\frac{1}{N}\sum_{i=1}^{N}f(\mathbf{y},\mathbf{z})\right]^2}.\tag{12}$$

The extended version of the Sobol' method presented by Saltelli in [23]. It has an additional advantage of the reduced cost of evaluating S_y and S_y^{tot}. Namely, for calculation of all one-dimensional indices it uses $N(n+2)$ model evaluation rather than $N(2n+1)$ for the original Sobol' formulas. Moreover, it was shown in [23] that these $N(n+2)$ model evaluations can be used for computing all two-dimensional indices. The extended version is based on using a different set of function values, namely $f(\mathbf{x}),f(\mathbf{x}'),f(\mathbf{y},\mathbf{z}')$.

One can notice that for less important variables values of the terms in nominator of (12) can be very close. It can result in the significant loss of accuracy. Situation can be improved using modified formula for S_y. It is easy to see that $f_0^2=(\int_{H^n}f(\mathbf{x})\,dx)^2=(\int_{H^n}f(\mathbf{x})\,dx)(\int_{H^n}f(x')\,dx')$. Hence, formula (10) can be rewritten as

$$S_y\approx\frac{\int_{H^n}f(\mathbf{x})f(\mathbf{y},\mathbf{z}')\,d\mathbf{x}\,dz'-(\int_{H^n}f(\mathbf{x})\,d\mathbf{x})(\int_{H^n}f(x')\,d\mathbf{x}')}{\int_{H^n}f^2(\mathbf{x})\,d\mathbf{x}-f_0^2}.\tag{13}$$

This expression can be reformulated as

$$S_y\approx\frac{\int_{H^n}f(\mathbf{x})[f(\mathbf{y},\mathbf{z}')-f(\mathbf{x}')]\,d\mathbf{x}\,d\mathbf{x}'}{\int_{H^n}f^2(\mathbf{x})\,d\mathbf{x}-f_0^2}.\tag{14}$$

The correspondent Monte Carlo algorithm has a form

$$S_y\approx\frac{\frac{1}{N}\sum_{i=1}^{N}f(\mathbf{y},\mathbf{z})[f(\mathbf{y},\mathbf{z})-f(\mathbf{y}',\mathbf{z}')]}{\frac{1}{N}\sum_{i=1}^{N}f^2(\mathbf{y},\mathbf{z})-\left[\frac{1}{N}\sum_{i=1}^{N}f(\mathbf{y},\mathbf{z})\right]^2}.\tag{15}$$

The improved formula (15), which was suggested by Kucherenko in [24], is based on the same set of function values as the extended version suggested by Saltelli [23]. A comparison of the original and improved formulas presented in [24,25] shows that for small value indices the improved formula produces a few orders of magnitude more accurate results. A comprehensive discussion of computation of S_y^{tot} can be found in [36].

5. Effective dimensions

The ANOVA decomposition was used for the introduction of a notion of the effective dimension in [3]. Let $\Lambda=\{1,2,\ldots,n\}$ and $|\mathbf{y}|$ be a cardinality of a set $\mathbf{y}\subseteq\Lambda$.

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

$$\sum_{0<|y|<d_S}S_y\ge p,\tag{16}$$

where p is the threshold, $0<p<1$.

Condition (16) means that the function f 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 $\sum_{0<|y|<d_S}S_y$ in order to reach the target p. Another notion of the effective dimension was implicitly introduced in [6]. In [3] it was called the effective dimension in the truncation sense.

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

$$\sum_{0<y\subseteq\{1,2,\ldots,d_T\}}S_y\ge p.\tag{17}$$

In other words, the effective dimension d_T is the highest number of variables, which need to be included in the sum $\sum_{0<y\subseteq\{1,2,\ldots,d_T\}}S_y$ in order to reach the target p. The value d_S does not depend on the order in which the input variables are sampled, while d_T does. For the same p $d_S\le d_T$.

It was suggested 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), although no formal proof was given [3]. By reducing the effective dimension, a higher efficiency of QMC integration can be achieved. One example of such an approach is a simulation driven by Brownian motion. It was shown that by changing the order in which the

variables are sampled from the LDS the effective dimension can be reduced and thus the accuracy can be significantly improved [3].

A straightforward evaluation of the effective dimension from its definitions (16), (17) is not practical in the general case as it would require the calculation of all 2^n components $\sigma_y^2(f_y)$. A quasi-regression method suggested in [7] is less computationally expensive. A truncated orthogonal decomposition based on orthogonal polynomials is used for an indirect estimation of $\sigma_y^2(f_y)$. The method allows the separation of high and low order subcomponents of f_y. The lower frequency or smoother parts of the ANOVA components of an integrand f are known to be related to the accuracy of integration rules applied to f. This method is still difficult to use for the prediction of QMC efficiency and there are some unresolved numerical issues such as the possibility of the negative variance estimates.

Owen introduced a probability measure $\mu(y)$ on non-empty subsets $y \subseteq \{1,\ldots,s\}$, in which $\mu(y)$ is proportional to the variance contribution to f of the subset u of input variables of f [4]. If U is a random μ distributed subset, then its cardinality, denoted $|U|$, is a random variable. The distribution $\nu(\cdot)$ of the random variable $|U|$ is the dimension distribution of f. The effective dimension can be defined through a quantile of the dimension distribution $\nu(\cdot)$. Although such quantiles are hard to estimate, Owen considered several cases of additive and multiplicative test functions for which such quantiles can be explicitly calculated. Owen also introduced the notion of mean dimensions. A similar concept was also suggested and used in [26]. One of the advantages of using mean dimensions is that they do no depend on the arbitrary threshold level p. The mean dimension was computed for some commonly considered test functions. It was shown that many of these functions are sums or products of univariate functions and have very low effective dimension. To analyze a class of isotropic test functions introduced by Capstick and Keister [27], Owen linked Sobol' SI with the dimension distribution. It allowed him to show numerically that the function classes under consideration are in fact very nearly a superposition of functions of 3 or fewer variables. Owen also noticed that low effective dimension is not sufficient to state that QMC will be more efficient than MC for discontinuous functions or functions with spikes such as some of Genz's functions. This observation is in accordance with earlier findings made in [14].

The set of variables $\mathbf{z}$ can be regarded as not important if $S_z^{tot} \ll 1$. In this case it is possible to fix a value of $\mathbf{z}$ at some nominal point $\mathbf{z}_0$ and to use $f(\mathbf{y},\mathbf{z}_0)$ as an approximation to $f(\mathbf{x})$. The approximation error depends on the choice of $\mathbf{z}_0$:

$$\delta(\mathbf{z}_0) = \frac{1}{\sigma}\int [f(\mathbf{x}) - f(\mathbf{y},\mathbf{z}_0)]^2\, d\mathbf{x}. \tag{18}$$

The following theorem shows that $\delta(\mathbf{z}_0)$ is of the same order as S_z^{tot}.

Theorem 1. *For an arbitrary $\mathbf{z}_0$ the error $\delta(\mathbf{z}_0) \geq S_z^{tot}$. If $\mathbf{z}_0$ is assumed to be random and uniformly distributed, then the expected value is*

$$\mathbf{E}\delta(\mathbf{z}_0) = 2S_z^{tot}. \tag{19}$$

Proof of this theorem can be found in [25]. A corollary of the theorem is the following assertion from [17]: for an arbitrary $\varepsilon > 0$ with probability exceeding $1-\varepsilon$

$$\delta(\mathbf{z}_0) < \left(1 + \frac{1}{\varepsilon}\right) S_z^{tot}. \tag{20}$$

Consider set $\mathbf{y} = (x_1,\ldots,x_d), 1 \leq d \leq n$ and a complimentary set $\mathbf{z} = (x_{d+1},\ldots,x_n)$. Using equality $S_z^{tot} = 1 - S_y$ and (17) for $d_T = d$ it is easy to see that

$$S_z^{tot} \leq 1 - p, \tag{21}$$

hence

$$\mathbf{E}\delta(\mathbf{z}_0) \leq 2(1-p). \tag{22}$$

6. Classification of functions based on Sobol' SI

Functions with respect to their dependence on variables can broadly be divided into two categories: functions with not equally important variables and functions with equally important variables. Functions with equally important variables according to the relationship between the values of S_i and S_i^{tot} can be further divided into two subgroups. Altogether, three different types of functions can be distinguished:

Type A: Functions with not equally important variables. Such functions are characterized by the small effective dimension d_T (and small d_S because of the condition: $d_S \leq d_T$). In terms of Sobol' SI, this case can be written as

$$\frac{S_y^{tot}}{n_y} \gg \frac{S_z^{tot}}{n_z}. \tag{23}$$

Here $\mathbf{y}$ is a group of leading variables, $\mathbf{z}$ is a group of complimentary variables, n_y, n_z are the number of variables in groups $\mathbf{y}$ and $\mathbf{z}$ correspondingly, $n_z = n - n_y$.

Type B: Functions with dominant low-order terms. Such functions are characterized by the small effective dimension $d_S \ll n$. In an extreme case of $d_S = 1$

$$S_i = S_i^{tot}, \quad 1 \leq i \leq n. \tag{24}$$

As a result

$$\sum_{i=1}^{n} S_i = 1$$

and $S_i = 1/n$.

Type C: Functions with dominant high-order interaction terms. Such functions are characterized by the high effective dimension $d_S \approx n$. For such functions

$$S_i < S_i^{tot}, \quad 1 \leq i \leq n. \tag{25}$$

This condition can also be written as

$$\sum_{i=1}^{n} S_i < 1.$$

This classification is summarized in Table 1.

Type A functions are probably the most common type of functions encountered in practice. For this case QMC can attain the rate of convergence $O(N^{-\alpha})$ with $\alpha \approx 1$, although the presence of high-order interaction terms can somewhat decrease the convergence rate.

Table 1
Classification of functions based on Sobol' sensitivity indices.

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

In the ANOVA decomposition of type B functions, the effective dimension d_S is small. In the extreme case it is equal to 1, and a function $f(\mathbf{x})$ can be presented as a sum of one-dimensional functions

$$f(\mathbf{x}) = \sum_{i=1}^{n} f_i(x_i).$$

QMC would always outperform MC for type B functions irrespective of the nominal dimension n. Although additive or nearly additive integrands are not very common, there are important application areas such as financial mathematics where such integrands are typical.

For type C functions both of the effective dimensions are equal or nearly equal to a nominal dimension n. For this type of functions QMC will lose its advantage over MC in high dimensions because of the importance of high-order terms in the ANOVA decomposition.

The evaluation of all main and total effects Sobol sensitivity indices for type B and C functions requires $N(n+2)$ function calculations. Computational costs can be further reduced by using the RS/QRS-HDMR method in which case the number of function evaluations is equal to N.

The identification of the effective dimension d_T for type A functions may require a few iterations before a set of non-important variables z satisfying condition (21) is found.

7. Numerical results

7.1. Path integrals

Consider the Wiener path integral

$$I = \int_C F[x(t)]\, d_\xi x, \tag{26}$$

where C is the space of all functions $x(t)$ continuous in the interval $0 \le t \le T$ with a boundary condition $x(0) = x_0$. The integral (26) can be regarded as an expectation with respect to the Wiener measure on C, so that $I = E(F[\xi(t)])$. Here $\xi(t)$ is a random Wiener processes (also known as a Brownian motion). A Monte Carlo approach consists of constructing many random paths $\xi(t)$, computing $F[\xi(t)]$ and averaging the results. We consider two discretization algorithms for random paths $\xi(t)$ generation. The first one is known as the standard discretization algorithm. It follows directly from the definition of $\xi(t)$. The second one is the alternative discretization algorithm also known as the Brownian bridge. It is based on the use of conditional distributions. Both algorithms were described in [28,29]. The alternative discretization algorithm was later analyzed in [30] within the framework of the quasi-Monte Carlo approach. Both algorithms have the same variance, hence their Monte Carlo accuracies are also the same but the corresponding quasi-Monte Carlo algorithms have different efficiencies with the Brownian bridge having the much higher convergence rate (although there are functionals $F[x(t)]$ for which the Brownian bridge does not offer a consistent advantage in quasi-Monte Carlo integration [31]).

Consider a functional

$$F[x(t)] = \int_0^T x^2(t)\, dt. \tag{27}$$

This integral can be evaluated analytically. We assume that the diffusion constant in the definition of Wiener's measure is $\frac{1}{2}$ and that boundary value $x(t) = x_0$ is fixed. The interval $0 \le t \le T$ is divided into n equal parts. It is assumed that $n = 2^l$, l is an integer number $l > 0$. Random values of the process at the moments of time $t_i = (i/n)T$, $1 \le i \le T$ are sampled by using independent normal $N(0;1)$ variable Z. A continuous path $x(t)$ is replaced with a polygonal approximation $x_n(t)$, details can be found elsewhere [29].

The expression for F_n has the general form

$$F_n = \sum_{i=0}^{n} a_i Z_i^2 + \sum_{i=0}^{n}\sum_{j<i}^{n} a_{ij} Z_i Z_j, \tag{28}$$

where Z_i are independent normal random variables, a_i and a_{ij} are coefficient values which depend on the type of approximation for $x_n(t)$. Applying global sensitivity analysis it is easy to show that the first and second order SI are given by

$$S_i = 2\frac{a_i^2}{\sigma^2(F_n)}, \quad S_{ij} = \frac{a_{ij}^2}{\sigma^2(F_n)}, \tag{29}$$

while all higher order SI are equal to zero. Here $\sigma^2(F_n)$ is the variance

$$\sigma^2(F_n) = 2\sum_i a_i^2 + \sum_{i<j} a_{ij}^2. \tag{30}$$

$\sigma^2(F_n)$ has the same value for both algorithms, so they are equivalent as far as the Monte Carlo method is concerned.

The results of the analytical evaluation of coefficients a_i show for the standard discretization coefficients a_i linearly decrease with the index number i. For the Brownian bridge discretization sensitivity indices of the first few variables are much larger than those of the subsequent variables. They also decrease more rapidly than sensitivity indices for the standard discretization. For the Brownian bridge the first two sensitivity indices are considerably larger than ones for the standard method. It results in particular in the much higher value of the sum of the first order sensitivity indices $\sum_i S_i$ for the Brownian bridge discretization than that for the standard discretization (Table 2). The results show for the standard approximation $\sum_i S_i$ decreases with the increase of the number of discretization points n approximately as $2/n$. As a result the importance of the second order interactions grows with n. They become dominant at $n > 4$. In contrast, for the Brownian Bridge approximation $\sum_i S_i$ is much higher than that of the second order indices $\sum S_{ij}$ and it is practically independent of the number of discretization points n. Table 2 also shows the effective dimensions. The effective dimension in the superposition sense is equal to 2 for both approximations irrespective of n. The effective dimension in the truncation sense is estimated using relationship (22) and values of S_z^{tot}. In Table 2 the following notation is used: $S_z^{tot}(d_T)$ is a value of S_z^{tot} for a set $z = (x_{d_T+1}, \ldots, x_n)$. For the Brownian Bridge approximation $d_T = 2$ for any n and it belongs to the type A function. For the standard approximation d_T is close to n ($d_T \approx \frac{3}{4}n$), however because of the small effective dimension in the superposition sense it belongs to the type B functions.

Table 2
Sensitivity indices for the standard and Brownian Bridge approximations.

Index	Function	Measure	Numerical values	
			$n=8$	$n=32$
3A	Brownian	$\frac{S_1}{S_1^{tot}}$	0.72	0.70
	Bridge	$\sum S_i$	0.72	0.72
	approximation	$\sum S_{ij}$	0.28	0.28
	$\int_{H^n} x^2(t)dt$	$S_z^{tot}(d_T)$	0.09	0.10
		d_T	2	2
		d_S	2	2
4B	Standard	$\frac{S_1}{S_1^{tot}}$	0.17	0.06
	approximation	$\sum S_i$	0.25	0.062
	$\int_{H^n} x^2(t)dt$	$\sum S_{ij}$	0.77	0.94
		$S_z^{tot}(d_T)$	0.05	0.09
		d_T	6	22
		d_S	2	2

It is well known that the initial low-dimensional coordinates of the low discrepancy sequences (LDSs) are more uniformly distributed than the later high-dimensional coordinates [9,11]. The Brownian bridge construction uses the best coordinates from each n-dimensional vector point to determine most of the structure of a path and reserves the later coordinates to fill in fine details. In other words, the most important variables are determined with the best dimensions of LDSs. It results in a significantly improved accuracy of quasi-Monte Carlo integration. In contrast, the standard construction does not account for the specifics of LDSs distribution properties.

Numerical results for the convergence rates presented in [32] confirm that for the standard Monte Carlo method there is no difference between the two discretizations. On the other hand the Brownian bridge discretization method with the Sobol sequence provides significantly more accurate results than the standard discretization.

7.2. Test problems commonly used in quadrature

To test the classification presented above, QMC and MC integration methods were compared considering seven different test functions presented in Tables 3–5. All functions are defined in H^n. Their integral values are equal to 1. Most of the functions are known test functions used previously in [33,5,34] and some other papers for testing QMC integration methods. Functions 2A, 3B and 3C were used in [35,10] as test functions for global sensitivity analysis.

The measures $S_1, S_1^{tot}, S_1/S_1^{tot}$ and $\sum_{i=1}^{n} S_i$ were calculated analytically. Analytical and numerical results for selected dimensions ($n=2$, 10, 100) are presented in Tables 3–5.

For each of the considered functions, the root mean square error

$$\varepsilon = \left(\frac{1}{K}\sum_{k=1}^{K}(I[f]-I_k[f])^2\right)^{1/2}$$

averaged over 50 runs ($K=50$) is presented in Figs. 1–3 as a function of N. For the MC method all runs were statistically independent. For QMC integration for each run a different part of the Sobol' LDS was used.

For practical purposes, MC and QMC integration errors can be approximated as

$$cN^{-\alpha}. \tag{31}$$

The exponents for the exponential decay α in (31) for QMC and MC integrations were extracted from the trend lines. The trend lines and corresponding values for $(-\alpha)$ are presented in Figs. 1–3.

The ANOVA decomposition for function 1A has the following form (for simplicity, a three-dimensional case is considered):

$$\begin{aligned} f(x_1,x_2,x_3) &= -x_1+x_1x_2-x_1x_2x_3 \\ &= f_0+f_1(x_1)+f_2(x_2)+f_3(x_3)+f_{1,2}(x_1,x_2)+f_{1,3}(x_1,x_3) \\ &\quad +f_{2,3}(x_2,x_3)+f_{1,2,3}(x_1,x_2,x_3) \end{aligned}$$

Table 3
Sensitivity indices for type A functions.

Index	Function $f(\underline{x})$	Ref.	Measure	Analytical values	Numerical values		
					$n=2$	$n=10$	$n=100$
1A	$\sum_{i=1}^{n}(-1)^i\prod_{j=1}^{i}x_j$	[5]	$\frac{S_1}{S_1^{tot}}$	$\frac{12}{27}\frac{(1-(-\frac{1}{2})^n)^2}{\frac{1}{2}-\frac{4}{5}(-\frac{1}{2})^n+\frac{3}{10}(\frac{1}{3})^n}$	0.75	0.89	0.89
			$\sum S_i$	[−]	0.86	0.89	0.89
2A	$\prod_{i=1}^{n}\frac{\lvert 4x_i-2\rvert+a_i}{1+a_i}$,	[35]	$\frac{S_1}{S_1^{tot}}$	$\frac{(1+D)^{(2-n)}}{(1+C)}$	–	0.71	0.0004
	$a_1=a_2=0$,		$\sum S_i$	$\frac{2C+(n-2)D}{(1+C)^2(1+D)^{(n-2)}-1}$	–	0.84	0.003
	$a_3=\cdots=a_{100}=6.52$			$C=\frac{1}{3(a_1+1)^2}, D=\frac{1}{3(a_3+1)^2}$			

Table 4
Sensitivity indices for type B functions.

Index	Function $f(\underline{x})$	Ref.	Measure	Analytical values	Numerical values		
					$n=2$	$n=10$	$n=100$
1B	$\prod_{i=1}^{n}\frac{n-x_i}{n-0.5}$	[34]	$\frac{S_1}{S_1^{tot}}$	$\left(\frac{1}{1+\frac{1}{12(n-0.5)^2}}\right)^{n-1}$	0.96	0.992	0.999
			$\sum S_i$	$\frac{n}{12(n-\frac{1}{2})^2\left[\left(1+\frac{1}{12(n-\frac{1}{2})^2}\right)^n-1\right]}$	0.981	0.995	0.999
2B	$\left(1+\frac{1}{n}\right)^n\prod_{i=1}^{n}\sqrt[n]{x_i}$	[34]	$\frac{S_1}{S_1^{tot}}$	$\left(1+\frac{1}{n^2+2n}\right)^{1-n}$	0.88	0.93	0.99
			$\sum S_i$	$\frac{n}{(n^2+2n)\left[\left(1+\frac{1}{n^2+2n}\right)^n-1\right]}$	0.941	0.963	0.995
3B	$\prod_{i=1}^{n}\frac{\lvert 4x_i-2\rvert+a_i}{1+a_i}$,	[35]	$\frac{S_1}{S_1^{tot}}$	$\left(1+\frac{1}{3(a_i+1)^2}\right)^{(1-n)}$	0.99	0.95	0.55
	$a_i=6.52$		$\sum S_i$	$\frac{n\frac{1}{3(a_i+1)^2}}{\left(1+\frac{1}{3(a_i+1)^2}\right)^n-1}$	0.99	0.97	0.74

Table 5
Sensitivity indices for type C functions.

Index	Function $f(\underline{x})$	Ref.	Measure	Analytical values	Numerical values		
					$n=2$	$n=10$	$n=100$
1C	$\prod_{i=1}^{n} \lvert 4x_i-2\rvert$	[33]	$\frac{S_1}{S_1^{tot}}$	$(\frac{4}{3})^{1-n}$	0.75	0.075	4.3×10^{-13}
			$\sum S_i$	$\frac{n}{3((\frac{4}{3})^n-1)}$	0.86	0.20	1.06×10^{-11}
2C	$(2)^n \prod_{i=1}^{n} x_i$	[-]	$\frac{S_1}{S_1^{tot}}$	$(\frac{3}{4})^{(n-1)}$	0.75	0.075	4.28×10^{-13}
			$\sum S_i$	$\frac{n}{3((\frac{4}{3})^n-1)}$	0.86	0.20	1.07×10^{-11}

$$= -\frac{3}{8} + \left(-\frac{3}{4}x_1 + \frac{3}{8}\right) + \left(-\frac{1}{8} + \frac{1}{4}x_2\right) + \left(\frac{1}{8} - \frac{1}{4}x_3\right) + \left(-\frac{1}{4}x_1 - \frac{1}{4}x_2 + \frac{1}{2}x_1x_2 + \frac{1}{8}\right) + \left(\frac{1}{4}x_1 + \frac{1}{4}x_3 - \frac{1}{2}x_1x_3 - \frac{1}{8}\right) + \left(\frac{1}{4}x_2 + \frac{1}{4}x_3 - \frac{1}{2}x_2x_3 - \frac{1}{8}\right) + \left(-\frac{1}{4}x_1 - \frac{1}{4}x_2 - \frac{1}{4}x_3 + \frac{1}{2}x_1x_2 + \frac{1}{2}x_1x_3 + \frac{1}{2}x_2x_3 - x_1x_2x_3 + \frac{1}{8}\right).$$

One can see by comparing $f_1(x_1)$, $f_2(x_2)$ and $f_3(x_3)$ that the variable x_1 is more important in terms of its variance than x_2 and x_3. It is also important to notice that first order terms are more important than interaction ones: the ratio S_i/S_i^{tot} is close to one both in low and high dimensions. $\sum_{i=1}^{n} S_i$ is also close to one (the analytic values for sensitivity indices for arbitrary i are given in [36]). To check condition (23), $S_{1,2}^{tot}$ and $S_{3,4,\ldots,200}^{tot}$ were calculated for $n=200$. Their values are $S_{1,2}^{tot}=0.94$ and $S_{3,4,\ldots,200}^{tot}=0.1$, hence $d_T=2$ assuming that $p=0.9$. These results confirm that condition (24) is satisfied, in which case QMC should be more efficient than MC irrespective of dimensionality. Indeed, the results of numerical integration confirm this prediction (Fig. 1a): for a high-dimensional problem with $n=360$, the exponent for algebraic decay $\alpha_{QMC}=0.94$ in (31) is only marginally smaller than theoretically predicted asymptotical value $\alpha_{QMC}=1.0$. The constant c is lower for the QMC method.

Function 2A in Table 3 was widely used in papers on global sensitivity analysis, where it was called "g-function" [35,10]. It can be seen that, as the value of a_i increases, the importance of the corresponding variable decreases. By varying values of a_i it is possible to change the type of the g-function. Three different sets of $\{a_i\}$ were engineered in such a way that all three types of functions were considered. For function 2A at $n=2S_{1,2}^{tot}=S_{3,4,\ldots,100}^{tot}=0.64$, so condition (23) is satisfied and d_T is close to 2. At the same time the interaction terms are dominant: $\sum_{i=1}^{n} S_i \approx 0$. The efficiency of QMC is still higher than that of MC at $n=100$, although α_{QMC} is only equal to $\approx$ 0.7 (Fig. 1b) and the constants c in (31) are almost equal for both methods.

All considered test functions with equally important variables are in fact symmetrical with regard to their variables

$$f(\ldots x_i,\ldots,x_j,\ldots)=f(\ldots x_j,\ldots,x_i,\ldots),\quad \forall\{i,j\},i\neq j.$$

Type B functions 1B and 2B (see Table 4) have very similar values of S_i/S_i^{tot} and $\sum_{i=1}^{n} S_i$ (both being very close to one). Fig. 2a and b confirm that the integration errors for both functions exhibit a similar behavior with QMC outperforming MC by several orders of magnitude at $n=360$.

With all a_i being equal to 6.52, the g-function becomes a type B function (function 3B in Table 4). The analysis of the global SI shows that for this function the interaction terms (although not being dominant) become more important at high n (S_i/S_i^{tot} decreases from 0.99 at $n=2$ to 0.55 at $n=100$). The values of the integration errors for the QMC and MC methods are very similar up to $N^*\approx 2^{16}$. At $N>N^*$ QMC becomes more efficient than MC (Fig. 2c).

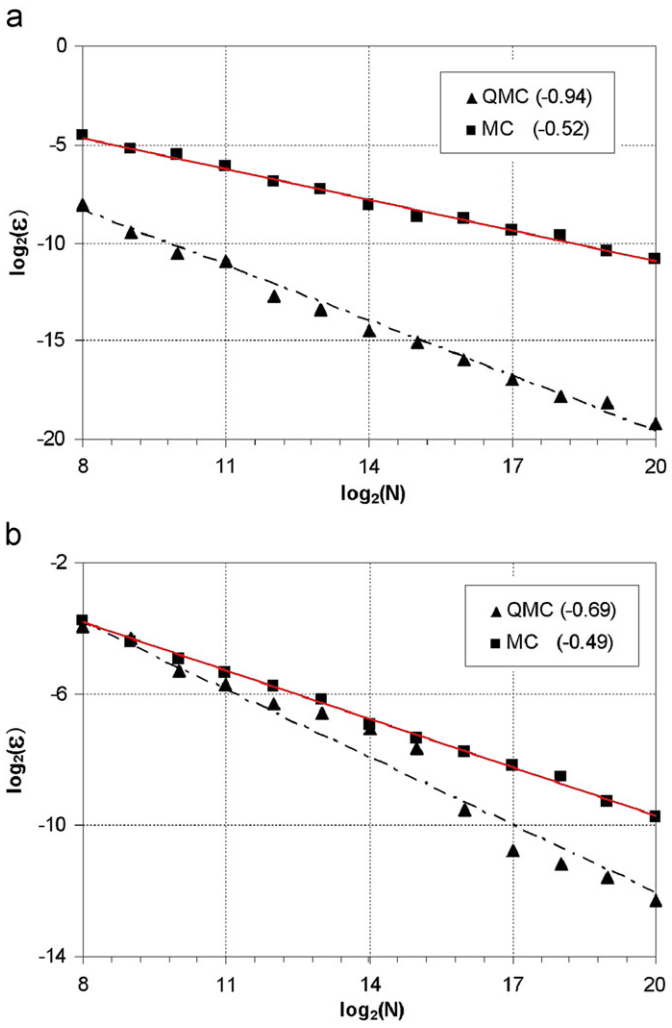

Fig. 1. The integration error ε vs. the number of sampled points. (a) Function 1A ($n=360$), (b) function 2A ($n=100$).

For functions 1C and 2C the ratio of S_i/S_i^{tot} rapidly decreases to 0 with n, which means that the higher order terms become dominant. The effective dimensions for such functions are equal to their nominal values. In this case, QMC loses its advantage over MC in high dimension. In particular, $\alpha_{QMC}\approx\alpha_{MC}$. The results presented in Fig. 3 confirm this prediction.

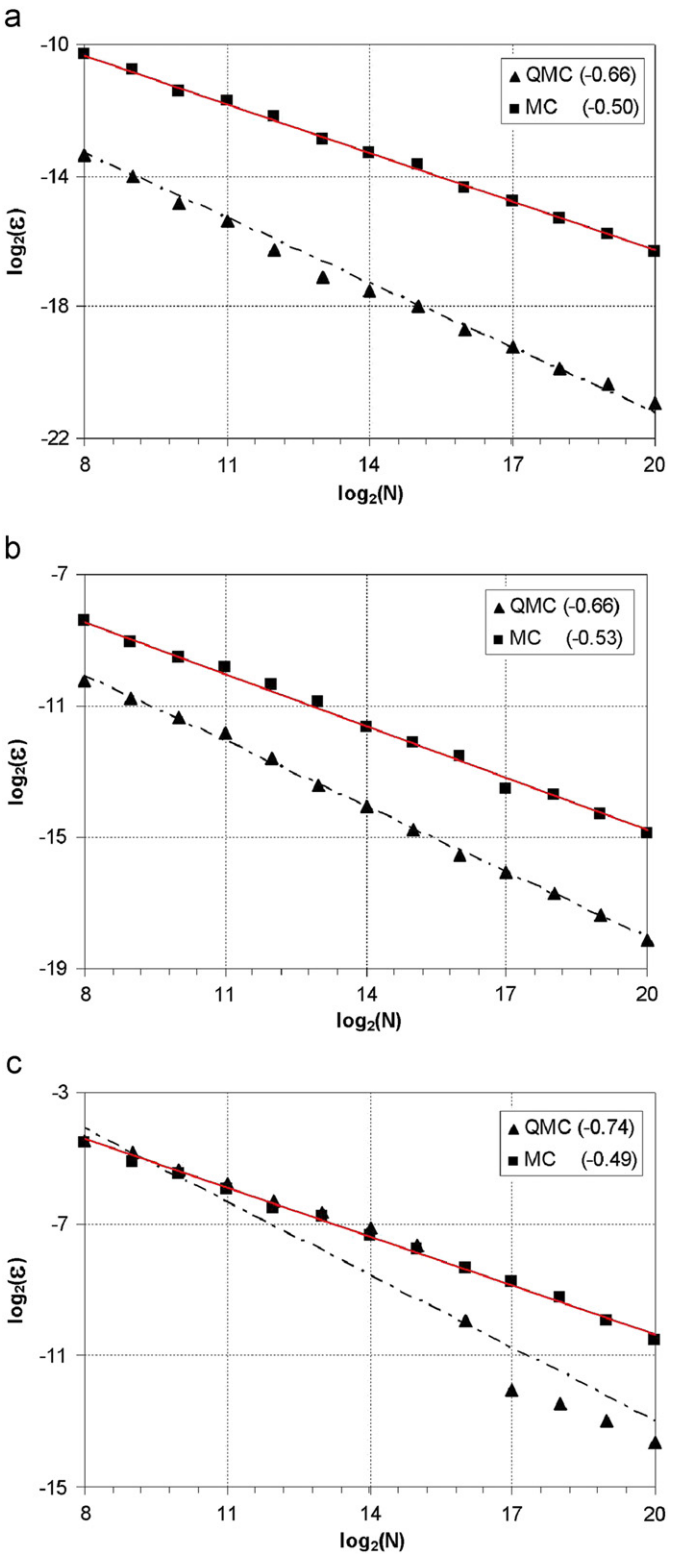

Fig. 2. The integration error ε vs. the number of sampled points. (a) Function 1B ($n = 360$), (b) function 2B ($n = 360$), (c) function 3B ($n = 100$).

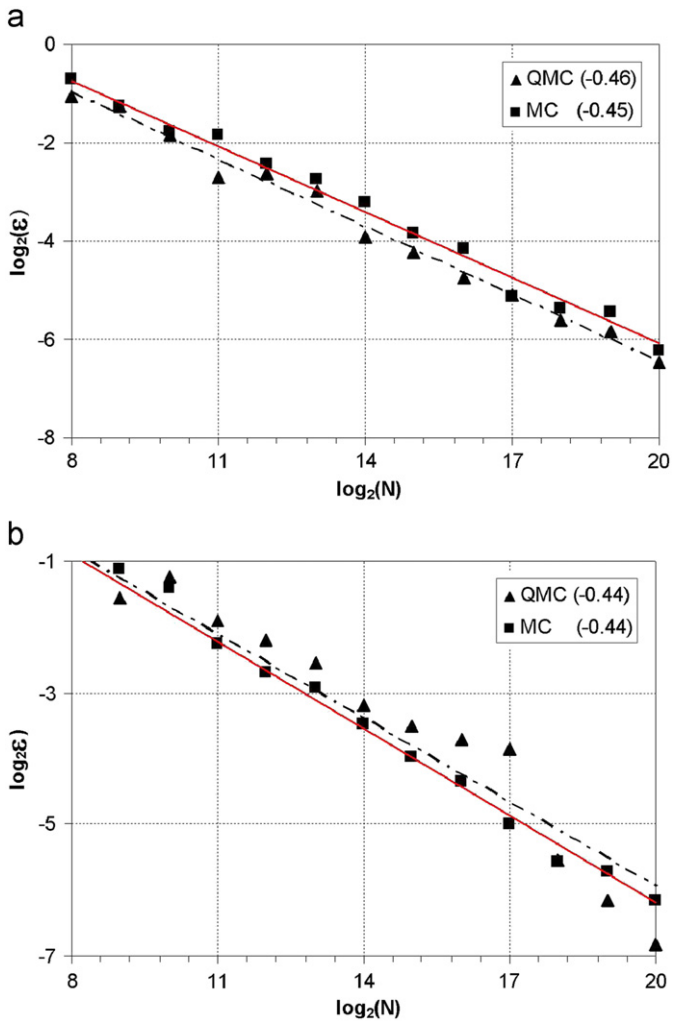

Fig. 3. The integration error ε vs. the number of sampled points. (a) Function 1C ($n = 20$), (b) function 2C (n = 20).

8. Conclusions

It has been shown that global sensitivity analysis allows the estimation of the effective dimensions at reasonable computational costs. Namely, d_T can be found by calculation of the Sobol' sensitivity indices for subsets of variables. d_S can be estimated by either using calculating the first order effects and the total Sobol' SI or by using the RS/QMC-HDMR method.

Global sensitivity analysis can also be used to predict the efficiency of the QMC method. Functions with respect to their dependence on the input variables can be loosely divided into three categories: functions with not equally important variables (type A) for which $d_T \ll n$; functions with equally important variables and with dominant low-order terms (type B) for which $d_S \ll n$, and functions with equally important variables and with dominant interaction terms (type C) for which $d_S = d_T = n$. For functions of type A and B, QMC is even in the high-dimensional case superior to MC while for functions of type C, QMC loses its advantage over MC because of the importance of higher order terms in the corresponding ANOVA decomposition. The results of numerical tests verify the prediction of the suggested classification.

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