Application of the control variate technique to estimation of total sensitivity indices

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A B S T R A C T

Global sensitivity analysis is widely used in many areas of science, biology, sociology and policy planning. The variance-based methods also known as Sobol’ sensitivity indices has become the method of choice among practitioners due to its efficiency and ease of interpretation. For complex practical problems, estimation of Sobol’ sensitivity indices generally requires a large number of function evaluations to achieve reasonable convergence. To improve the efficiency of the Monte Carlo estimates for the Sobol’ total sensitivity indices we apply the control variate reduction technique and develop a new formula for evaluation of total sensitivity indices. Presented results using well known test functions show the efficiency of the developed technique.

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1. Introduction

Global sensitivity analysis (SA) is the study of how the uncertainty in model output is apportioned to the uncertainty in model inputs [1,2]. Over the last decade, global SA has gained acceptance among practitioners in the process of model development, calibration and validation, reliability and robustness analysis, decision-making under uncertainty, quality-assurance, and complexity reduction. There have been many successful improvements in the efficiency of estimating the main effect Sobol’ indices ranging from the advanced formulas for small sensitivity indices [3,4] to application of RBD [5] and various metamodelling methods [6–11]. However, there have been no similar advances concerning estimation of the total sensitivity indices and the Sobol-Jansen formula [12,13] remains to be the only formula used in the direct computation of the total sensitivity indices.

To improve the efficiency of the Monte Carlo (MC) estimates for total sensitivity indices we apply the variance reduction technique and develop a new formula for the evaluation of total sensitivity indices. We also present results using well known test functions to show the efficiency of the developed technique.

This paper is organised as follows. The next section introduces control variates reduction technique. ANOVA decomposition and Sobol’ sensitivity indices are briefly presented in Section 3. In Section 4 we describe how to apply the control variate technique to improve the efficiency of the Sobol-Jansen formula for evaluation of total sensitivity indices. The use of metamodels is presented in Section 5. This section also provides the details of the random sampling-high dimensional model representation (RS-HDMR) model which is used in this paper. Four different test cases are considered in Section 6. Finally, conclusions are shown in Section 7.

2. Control variate reduction technique

Consider the integral of the function $f$ over the $n$-dimensional unit hypercube $H^n$:

$$I[f] = \int f(x) dx.$$ 

This integral can be seen as an expectation of $f(x)$ with respect to an $n$-dimensional random variable $x$ that is uniformly distributed:

$$I[f] = E[f(x)] = \int f(x) dx. \quad (1)$$

Further we denote $\mu_f = E[f(x)]$. To calculate this expectation, a sequence of $N$ random or quasi random points $x^{(i)}$ is sampled and then the mathematical expectation (1) is approximated as follows:

$$I_N[f] = \frac{1}{N} \sum_{i=1}^{N} f(x^{(i)}) \quad (2)$$

It is important to estimate an integration error $\varepsilon = |I[f] - I_N[f]|$. For the MC method the expectation of $\varepsilon^2$ is equal to $\sigma^2(f)/N$.
where \( \sigma^2 = \text{Var}[f] \) and the root mean square error \( \varepsilon_{\text{MC}} = \sigma / \sqrt{N} \). To reduce \( \varepsilon_{\text{MC}} \) one can either increase the number of sampled points \( N \), or to decrease the variance \( \sigma^2 \). The objective of this paper is to develop a new efficient formula for evaluation of total sensitivity indices based on the reduction of the variance of its MC estimate. There are various variance reduction techniques used to increase the accuracy of the MC estimates [14]. One of them is the control variate method which we further consider.

To improve the MC estimate of \( \mu_f \) we define a new function \( \tilde{f}(x) \):

\[
\tilde{f}(x) = f(x) + C(g(x) - \mu_g),
\]

where \( C \) is a constant coefficient, \( g(x) \) is a function known as a control variate for which an expectation \( \mu_g = \int g(x)dx \) is known. It is easy to see that \( \text{E}[\tilde{f}(x)] \) is an unbiased estimator for \( \mu_f \) for any choice of the coefficient \( C \): \( \text{E}[\tilde{f}(x)] = \text{E}[f(x)] \) as \( \text{E}[C(g(x) - \mu_g)] = 0 \).

Consider the variance of the resulting estimator \( \tilde{f} \):

\[
\text{Var}[	ilde{f}] = \text{Var}[f] + C^2 \text{Var}[g] + 2C \text{Cov}[f, g] \tag{4}
\]

The main objective is to make sure that \( \text{Var}[	ilde{f}] \leq \text{Var}[f] \). Minimum of (4)

\[
\min_{C} \text{Var}[	ilde{f}]
\]

is attained at \( C = C^* \):

\[
C^* = - \frac{\text{Cov}[f, g]}{\text{Var}[g]}. 
\]

In this case

\[
\text{Var}[	ilde{f}] = \text{Var}[f] - \frac{\text{Cov}^2[f, g]}{\text{Var}[g]}. 
\]

The root mean square error \( \varepsilon_{\text{MC}} \) is then equal to \( \text{Var}[	ilde{f}] / N^{0.5} \). The difficulty here is to find a good control variate \( g \) to build an unbiased estimator \( \tilde{f} \) with a reduced variance.

### 3. Sobol’ sensitivity indices

The method of global sensitivity indices is based on the decomposition of a function into summands of increasing dimensionality. Consider an integrable function \( f(x) \) defined in the unit hypercube \( H^n \). It can be expanded in the following form:

\[
f(x) = f_0 + \sum_{j=1}^n f_j(x_j) + \sum_{0 \leq i < j \leq n} f_{i,j}(x_i, x_j) + \ldots + f_{1,\ldots,n}(x_1, \ldots, x_n). \tag{5}
\]

Each of the components \( f_{0,\ldots,k}(x_1, \ldots, x_k) \) is a function of a unique subset of variables from \( x \). It can be proven [12,13] that the expansion (6) is unique if

\[
\int_0^1 f_{1,\ldots,k}(x_1, \ldots, x_k) dx_k = 0, \quad 1 \leq k \leq s,
\]

in which case it is called a decomposition into summands of different dimensions. This decomposition is also known as the ANOVA decomposition.

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

\[
D = \sum_{s=1}^n \sum_{l_1 < \ldots < l_s} D_{l_1,\ldots,l_s}.
\]

Here \( D = \text{Var}[f] \) is the total variance, \( D_{l_1,\ldots,l_s} \) are partial variances defined as

\[
D_{l_1,\ldots,l_s} = \int_0^1 f_{l_1,\ldots,l_s}(x_1, \ldots, x_s) dx_l_1, \ldots, x_l_s
\]

We note that is customary in the area of global sensitivity indices to use \( D \) to denote the variance instead of \( \text{Var}[f] \) which is more common in statistics.

Sobol’ main effect sensitivity indices are defined as the ratios

\[
S_{i_1,\ldots,i_s} = D_{i_1,\ldots,i_s} / D.
\]

Consider two complementary subsets of variables \( x_j \) and \( x_{-j} \), where \( x_{-j} \) is \( n-1 \) dimensional vector. The total variance \( D_j \) is defined as

\[
D_j = D - D_{-j},
\]

where \( D_{-j} \) is the sum of all the marginal variances not containing \( j \) in their subscripts. The corresponding total sensitivity indices [11,12] are equal to

\[
S_j = D_j / D.
\]

Obviously, \( S_j = S - S_{-j} \), where \( S_{-j} = D_{-j} / D \). Knowledge of \( S_j \) and \( S_{-j} \) in most cases provides sufficient information to determine the sensitivity of the analysed function to individual input variables.

Sobol’ sensitivity indices can be computed using direct formulas [12,13]. Significant progress has been made in improving efficiencies of computing main effect indices [5]–[3]. In the next section we propose a new efficient approach to compute total sensitivity indices.

### 4. Application of the control variate technique to estimation of total sensitivity indices

We apply the control variate technique idea presented in Section 2 to the evaluation of the total sensitivity indices \( S_j \) for the case of a single variable \( x_j \). This approach can be easily generalized for the case of a set of variables.

The Sobol–Jansen formula has a form [12,13]:

\[
S_j = \frac{1}{2D} \int \left[ f(x) - f(x_j, x_{-j}) \right]^2 dx dx_j, \tag{6}
\]

where \( x_j \) is \( j \)-th component of the \( n \)-dimensional \( x \) vector which is sampled independently from \( x \). In this section we omit for brevity the integral limits.

Application of the control variate technique would require finding a new function (3), such that

\[
\tilde{f}(x, x_j) = f(x, x_j) + C(G(x, x_j) - \mu_g),
\]

where \( f(x, x_j) = \left[ f(x) - f(x_j, x_{-j}) \right]^2 \). \( \mu_G = \int G(x, x_j)dx dx_j \). It is not possible to find a control variate \( G(x, x_j) \) in a general case. However, a natural choice for the control variate for a function \( f(x) \) is to choose the first order terms of ANOVA

\[
g(x) = f_0 + \sum_{i=1}^n f_i(x_i). \tag{7}
\]

Similarly, a good control variate for \( f(x_j, x_{-j}) \) is

\[
g(x_j, x_{-j}) = f_j(x_j) + \sum_{i \neq j} f_i(x_i). \tag{8}
\]

**Theorem.** Approximating functions \( f(x) \) and \( f(x_j, x_{-j}) \) in (6) with (7) and (8) results in the following formula for \( S_j \):

\[
S_j = \frac{1}{2D} \int \left[ f(x) - f_j(x_j) - \left[ f(x_j, x_{-j}) - f_j(x_j) \right] \right]^2 dx dx_j + S_j. \tag{9}
\]

**Proof.** Consider function \( F_M = f(x) - f_j(x_j) - \left[ f(x_j, x_{-j}) - f_j(x_j) \right] \). Its variance is

\[
\text{Var}[F_M] = \int \left[ f(x) - f_j(x_j) - \left[ f_j(x_j) \right] \right]^2 dx dx_j
\]
Forty types and functions important variables and with dominant interaction terms (type C). makes this method more difficult by adding higher order terms to control variate, however it indices and the (typically second or third) because for many practical problems only between these methods is that RS-HDMR is based on cutting higher to the Polynomial Chaos Expansion (PCE) method [10]. The difference Sj and Z

As shown in [3] models with respect to their dependence on the input variables can be loosely divided into three categories: models with not equally important variables only a few of which are important (type A), models with equally important variables and with dominant low order terms (type B) and models with equally important variables and with dominant interaction terms (type C). For type A and B functions f(x) and f(x, x, ...) can be approximated with (7) and (8), respectively with sufficient accuracies.

The developed technique should provide a significant efficiency improvement for types A and B functions. For the type C functions Sj are much larger than Sj and hence the choice of fj(xj) as control variate is not sufficient as the higher order interaction terms play a significant role in the ANOVA decomposition of f(x).

5. The use of metamodels

The developed technique requires that the first order ANOVA terms fj(xj) and the corresponding Sj to be known explicitly. In a general case of functions not known analytically fj(xj) and Sj can only be found by building metamodels and then extracting the numerical values of the first order sensitivity indices and approximation of the first order terms of the ANOVA decomposition from these metamodels. We applied the RS-HDMR method suggested in [9] to approximate fj and Sj in the formula (9), although it is possible to use other metamodeling methods: kriging, RBF, etc. [6-8]. The RS-HDMR method is similar to the Polynomial Chaos Expansion (PCE) method [10]. The difference between these methods is that RS-HDMR is based on cutting higher order terms in the ANOVA decomposition above a certain order (typically second or third) because for many practical problems only the low order terms in the ANOVA decomposition (5) are important, hence f(x) can be approximated by

\[ f(x) \approx f_0 + \sum_{i=1}^{d} \sum_{j<i, k} f_{ij} \phi_i(x) \phi_j(x) \]  

(11)

Here d is a truncation order, which for many practical problems can be equal to 2 or 3 [9]. The component functions in (11) are expanded in terms of a suitable set of functions depending on the distribution of input variables. Typically in the RS-HDMR and PCE methods orthonormal polynomials are used. Using a complete base of orthogonal polynomials \( \{\phi_i\} \) the first and second order terms are expanded as:

\[ f_j(x) = \sum_{r=1}^{\infty} \alpha_{rj} \phi_r(x), \quad f_{ij}(x) = \sum_{p=1}^{\infty} \sum_{q=1}^{\infty} \beta_{pqij} \phi_p(x) \phi_q(x). \]

(12)

Here \( \{\alpha_{rj}\} \) and \( \{\beta_{pqij}\} \) are the coefficients of decomposition which needs to be determined. Due to orthogonality of polynomials the first and second order sensitivity indices are defined using only the coefficients of the decomposition (12) as follows [10]:

\[ S_j = \frac{1}{D_j} \sum_{i=1}^{d} |\alpha_{ij}|^2, \quad S_{ij} = \frac{1}{D_p D_q} \sum_{p=1}^{\infty} \sum_{q=1}^{\infty} |\beta_{pqij}|^2. \]

(13)

In practice summations in (12) and (13) are limited to some maximum orders. Coefficients of decomposition \( \{\alpha_{rj}\} \) and \( \{\beta_{pqij}\} \) can be found using a regression method or MC or Quasi MC integration. The details of implementation can be found in [11], where a Quasi RS-HDMR (QRSHDMR) variant of the RS-HDMR method was developed. One of the distinctive characteristics of the QRSHDMR method is that Quasi MC sampling is used in the metamodel training set. In this work we used a regression method for determining the coefficients of decomposition.

6. Test cases

In this section we evaluate total sensitivity indices \( S_j^T \) for a set of functions with known analytical values for the first order sensitivity indices and the expressions for the first order terms of the ANOVA decomposition using the original formula (6) (which we further call standard) and the improved formula (9) using expressions for \( f_j(x_j) \) and \( S_j \) computed either analytically or applying the metamodeling technique. In each test case, the MC estimates of total sensitivity indices computed using formulas (6) and (9) are calculated for a number of sampled points \( N \) up to 215. In all cases we used MC sampling. We present results for the convergence of \( S_j^T \) and the root mean square error (RMSE) \( e_j(N) \) versus \( N \). RMSE is defined as:

\[ e_j(N) = \left[ \frac{1}{K} \sum_{k=1}^{K} \left( S_j^{\text{true}} - S_j^T \right)^2 \right]^{1/2}. \]

(14)

Here \( S_j^{\text{true}} \) is a numerical estimate of \( S_j^T \) at kth repetition, \( S_j^{\text{true}} \) is an analytical value of \( S_j^T \). For the MC method all runs should be statistically independent. In this work the number of independent repetitions \( K \) was equal to 20.

For each test case we also present histograms which graphically show the difference between the original and control variate reduction techniques. For all tests we present the histogram of the distribution of \( f(x) - f(x, x, ...) \) which is used in the standard formula (6) and the histogram of the distribution of \( f(x) - f_j(x_j) - f_j(x_j) - f_j(x_j) \) which is used in the formula (9). We give the values of the variance \( \text{Var} f_j \) for the standard formula (6) which corresponds to the distribution \( f(x) - f_j(x_j) \), the variance \( \text{Var} f_j \) for the control variate formula (9), which corresponds to the distribution \( f(x) - f_j(x_j) - f_j(x_j) - f_j(x_j) \) and their ratio \( \text{Var} f_j / \text{Var} f_j \). We note that values \( \text{Var} f_j \) and \( \text{Var} f_j \) depend on an input variable j.
6.1. Ishigami function

The Ishigami function is often used as a benchmark in sensitivity analyses studies [1]. This function is defined as:

\[ f(x) = \sin(x_1) + a \sin^2(x_2) + bx^4 \sin(x_1). \]

Here input factors \( x_j \) are uniformly distributed: \(- \pi \leq x_j \leq \pi, \) \( j = 1, 2, 3, \) parameters \( a = 7, \ b = 0.1. \) The first order terms of the ANOVA decomposition for this function are \( f_1(x_1) = \sin(x_1)(1 + \sin^2(x_2)) \), \( f_2(x_2) = a \sin^2(x_2) - a/2, \) \( f_3(x_3) = 0. \)

Table 1 presents analytical values of the first order and total indices. From the values of sensitivity indices one can see that strictly speaking it is neither type A nor type B function. However, for input 2 \( S_j^1 = S_2, \) hence the first term of the right hand side expression in (9) is equal to 0 and application of the control variate formula should show the dramatic increase in efficiency. One can also expect that formula (9) can give efficiency improvement for the first input. For the third input variable \( f_3(x_3) = 0 \) and \( S_3 = 0, \) hence there should be no difference in efficiencies of formulas (6) and (9).

Numerical tests confirm these assumptions. Total sensitivity indices \( S_j \) for the first and second input variables were computed using the original formula (6) and the improved formula (9). We used analytical expressions for both \( f_j(x_j) \) and \( S_j \) (curves noted as “reduction”) and expressions for \( f_j(x_j) \) and \( S_j \) obtained from a metamodel as described in Section 3 (curves noted as “HDMR reduction”). QRS-HDMR with \( N = 128 \) sampled points was used to build a metamodel and to approximate \( f_j \) and \( S_j. \) We note that from the efficiency point of view, metamodels should be constructed with the minimum possible number of function evaluations.

Figs. 1 and 2 show the results of convergence and RMSE of \( S_j^1, j = 1, 2, 3 \) versus the number of sampled points \( N \) for three different cases: standard formula (6), control variate formula (9) with using \( f_j(x_j) \) and \( S_j \) computed analytically, and \( f_j(x_j) \) and \( S_j \) based on metamodel computations. Control variate formula (9) with using \( f_j(x_j) \) and \( S_j \) computed either analytically or using metamodel gives a significant speed up in convergence for the first input (Fig. 1a), while for the second input it gives practically instantaneous convergence (Fig. 1b) as expected. For the third input for reasons given above there is no difference in convergence of all three methods (Fig. 1c).

It follows from Fig. 2a that for the first input the control variate formula gives improvements in convergence up to 3 folds, when analytical expressions for \( f_j(x_j) \) and \( S_j \) are used and up to 2 folds, when metamodel based expressions for \( f_j(x_j) \) and \( S_j \) are used. For the second input (Fig. 2b) in the case of analytically computed \( f_2(x_2) \) and \( S_2 \) indices \( S_j^1 = S_2 \) regardless of the number of sampled points. As a result, RMSE for this case is exactly equal to 0. In the case of \( f_2(x_2) \) and \( S_2 \) computed using metamodels, RMSE is many orders of magnitude smaller than that computed using the standard formula. For the third input RMSE for all three methods is the same (Fig. 2c). Hence we can conclude that the control variate formula does not give improvements in the case of inputs for which \( S_j \approx 0 \) and \( S_j^1 \) is relatively large.

Computation of variance for the first input for the original and control variate formulas gives the following results: \( V_j(j = 1) = 13.8, V_j(j = 1) = 5.8. \) The ratio \( V_j(j = 1)/V_j(j = 1) = 2.4. \) It also follows from the presented histogram in Fig. 3 that the control variate formula shows a decrease of the variance.

Table 1

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<th>Factor</th>
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<th>Total index</th>
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</tr>
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<td>2</td>
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<tr>
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</tr>
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6.2. G-function

The g-function is also used as a benchmark in global sensitivity analyses tests [12]. This function is defined as:

\[ f(x) = \prod_{j=1}^{n} g_j(x_j, a_j) = \prod_{j=1}^{n} \frac{|4x_j - 2| + a_j}{1 + a_j}. \]

Here \( n \) is the number of independent input factors \( x_j, 0 \leq x_j \leq 1, j = 1, \ldots, n. \) Further we consider a problem with \( n = 8 \)
input variables with the vector of parameter \( \{a_j\} = \{0, 1, 4.5, 9, 99, 99, 99, 99\} \). Parameter \( a_j \) is set to determine the importance of the input factor \( x_j \), given that the range of variation of \( g_j(x_j, a_j) \) depends exclusively on the value of \( a_j \). If \( a_j = 0 \), the corresponding input \( x_j \) is important; if \( a_j = 1 \), \( x_j \) is relatively important, while for \( a_j = 9 \) it becomes non-important and for \( a_j = 99 \) non-significant.

For this function the first order partial variances are equal to \( D_j = 1/3(1+ a_j)^2 \), the higher order partial variances are products \( D_{ij} = D_{hi}, \ldots, D_{j} \) and the total variance is \( D = \prod_{j=1}^{n} (D_j + 1) - 1 \). The first order terms of the ANOVA decomposition are \( f_j(x_j) = g_j(x_j, a_j) - 1, i = 1, \ldots, n \). Table 2 presents analytical values of the first order and total sensitivity indices. From the values of the first order and total sensitivity indices one can see that \( S^T_j \) is close to \( S_j \). This is a type A function, and hence the developed method should be efficient.

We note, that the g-function has a kink at \( x_j = 0.5, j = 1, \ldots, n \) and it is not differentiable at this point. Building metamodels for such functions using continuous smooth function as a decomposition base is especially difficult as it is not possible to approximate regions of the functions in the vicinity of kinks with sufficient local accuracy. QRS-HDMR with \( N=1024 \) sampled points was used to build a metamodel and to approximate \( f_j \) and \( S_j \). This number of sampled points is much higher than that used for the Ishigami function (\( N=128 \)) due to both the existence of a kink and higher dimensionality of the considered g-function (\( n=8 \) while for the Ishigami function \( n=3 \)).

The results for the convergence and RMSE of \( S^T_j, j = 1, 3, 5 \) versus the number of sampled points \( N \) for the standard formula (6) and the control variate formula (9) with using \( f_j(x_j) \) and \( S_j \) computed analytically and using a metamodel are presented in Figs. 4 and 5. Improvements in convergence with control variate formula (9) strongly depend on the value of \( S^T_j \): it is very significant for the first input with high values of \( S_j \) and \( S^T_j \) (Fig. 4a) and it is less significant for the third input with small values of \( S_j \) and \( S^T_j \) (Fig. 4b) for both analytically and metamodel computed \( f_j(x_j) \) and \( S_j \). However, for the fifth input there is only some improvement in convergence with \( f_j(x_j) \) and \( S_j \) computed analytically while in the case of metamodel based \( f_j(x_j) \) and \( S_j \) there is no convergence to the analytical value of \( S^T_j \) (Fig. 4). It is explained by the fact that for non-significant inputs with

<table>
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<td>1.0e-04</td>
<td>1.05e-04</td>
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extremely small values of $S_j$ and $S_T^j$ as in the case of inputs 5 to 8 it is practically not possible to compute $f_j(x_j)$ and $S_j$ with sufficient accuracy due to high metamodelling errors. We note, that this situation is different from the previous test case with the Ishigami function for which $S_j = 0$ but $S_T^j$ has a relatively large value.

Fig. 5 also confirms these findings: for the first input the control variate formula gives improvements in convergence up to 15 folds, for the third input it is approximately 4 folds for both analytically and metamodel based $f_j(x_j)$ and $S_j$. For the fifth input improvements in convergence is 4 folds for analytically given $f_j(x_j)$ and $S_j$ while for the metamodel based $f_j(x_j)$ and $S_j$ there is no convergence to the true value of $S_T^j$. We also notice that the values of RMSE drop many orders of magnitude with the increase of the input number.

Fig. 6 shows that switching from integrand $[f(x) - f(x_j, z)]$ to $f(x) - f(x_j) - [f(x_j, z) - f(x_j)]$ gives a dramatic decrease in the variance: for the first input $V_S(j=1) = 0.8$, $V_T(j=1) = 0.07$, the ratio $V_S(j=1)/V_T(j=1) = 11.4$.

Fig. 4. Convergence of $S_T^j$ for G-function. First input (a); third input (b); fifth input (c). Blue line: standard formula (6); red line: control variate reduction formula (9) with using analytically given $f_j(x_j)$ and $S_j$; green line: control variate reduction formula (9) with using $f_j(x_j)$ and $S_j$ based on metamodel computations; purple line: analytical values of $S_T^j$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 5. log$_2$(RMSE) vs. log$_2$(N) for G-function. First input (a); third input (b); fifth input (c). Blue line: standard formula (6); red line: control variate reduction formula (9) with using analytically given $f_j(x_j)$ and $S_j$; green line: control variate reduction formula (9) with using $f_j(x_j)$ and $S_j$ based on metamodel computations; purple line: analytical values of $S_T^j$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
We can conclude that the control variate formula does not give improvements in the case of inputs for which $S_j^1 \approx 0$.

6.3. Product function

Owen considered product functions of the following form [4]:

$$f(x) = \prod_{j=1}^{n} [\mu_j + \tau_j g_j(x_j)].$$

Here $g(x) = \sqrt{12(x - 0.5)}$. In this study, we use $n = 6$, $\{\tau_j\} = [1, 1, 0.5, 0.5, 0.25, 0.25]$ and $\mu_j = 1$ for all $j$. The total variance $D$ is $D = \prod (\mu_j^2 + \tau_j^2) - \prod \mu_i^2$. The first order terms of the ANOVA decomposition are

$$f_j(x_j) = [\mu_j + \tau_j g_j(x_j)] \prod_{i=1}^{n} (\mu_i) - \prod \mu_i.$$ 

The analytical values for first order and total sensitivity indices are:

$$S_j = \frac{1}{D} \left[ (\mu_j^2 + \tau_j^2) \prod_i \mu_i \right], \quad S_j^1 = \frac{1}{2D} \left[ 2\tau_j^2 \prod_i (\mu_i^2 + \tau_j^2) \right].$$

From the values of the first order and total sensitivity indices one can see (Table 3) that this is a type C function, $S_j^1$ are much larger than $S_j$ and hence the choice of $f_j(x_j)$ as a control variate is not sufficient as the higher order interaction terms play a significant role in the ANOVA decomposition of $f(x)$.

Fig. 7 shows that although both methods converge to the analytical values, there is no real improvement in applying the control variate method using only the first order terms $f_j(x_j)$. Plots of RMSE (Fig. 8) also show that there are no significant improvements in the use of the control variate method.

Comparison of the histograms also shows that there is no significant reduction of variance for a function of this type (Fig. 9): for the first input $V_S(j = 1) = 7.0$, $V_\mu(j = 1) = 5.0$, the ratio $V_S(j = 1)/V_\mu(j = 1) = 1.4$. Similar results were obtained for other inputs.

### 7. Conclusions

It was shown that the control variate reduction technique can be used to improve the efficiency of the Sobol–Jansen formula for evaluation of total sensitivity indices. The control variate reduction formula for total sensitivity indices requires the knowledge of the first order sensitivity indices and the first order terms of the ANOVA decomposition. They can be obtained either from

<table>
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<th>Table 3</th>
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<td>First order and total sensitivity indices. Owen’s product function.</td>
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<td>$S_j$, $j = 1, \ldots, 6$</td>
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<tr>
<td>$S_j^1$, $j = 1, \ldots, 6$</td>
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analytical exact expressions (in the case of explicitly given model functions) or from using metamodelling techniques, although the latter is more practical.

Presented results using well known test functions show high efficiency of the developed technique for types A and B functions. However, for type C functions the control variate reduction formula does not offer improved efficiency which is explained by the importance of higher order terms in the ANOVA decomposition for this type of functions.

In most cases a practitioner does not know in advance the type of functions. However, in practice it is possible to estimate main effect sensitivity indices with a limited number of function evaluations using recent advances in global sensitivity analysis and metamodelling. In the case of inputs for which $S_j \approx 0$ it is not advisable to use the control variate formula as it does not give improvements in the case of inputs for which $S_j \approx 0$ and $S_j^2$ is relatively large, while for non-significant inputs with extremely small values of $S_j$ and $S_j^2$ the control variate formula is less efficient than the Sobol–Jansen formula as it is practically not possible to compute the first order sensitivity indices and the first order terms of the ANOVA decomposition with sufficient accuracy due to high metamodelling errors.

The efficiency of the proposed method can be increased further by adding higher order terms to control variate approximation of the model function. However this would make the method less practical.

Finally, we note that it is important in practice to obtain confidence intervals associated with MC estimates (in our case in estimating total sensitivity index using the control variate technique). It can be done e.g. by using the bootstrap procedure [16] and its variants specially adapted for evaluation of sensitivity indices based on metamodels [17] or using Gaussian process formulation [18].

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