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GLOBAL SENSITIVITY ANALYSIS OF NONLINEAR MATHEMATICAL MODELS - AN IMPLEMENTATION OF TWO COMPLEMENTING VARIANCE-BASED ALGORITHMS

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ABSTRACT

A new approach for a global sensitivity analysis of nonlinear mathematical models is presented using the information provided by two complementing variance-based methods. As a first step, the model is evaluated applying a shared sampling strategy for both methods based on Sobol's quasi-random sequences. Then, total sensitivity indices are estimated in a second step using the Sobol'-Saltelli method whereas first-order sensitivity indices are concurrently computed using a modified version of the well-known Fourier Amplitude Sensitivity Test. Although the analysis is focused on the calculation of total sensitivity indices, first-order sensitivity indices and thus information about the main effects of model input parameters can be obtained at no extra computational cost. Another advantage of this approach is that data of previous model evaluations can be reused for a new, more precise sensitivity analysis. The capability and performance of the method is investigated using an analytical test function.

1 INTRODUCTION

In many fields of science and technology mathematical models are used for the simulation of different systems in order to understand and predict their potential behavior. However, the complexity of these models increased rapidly over the past years. One consequence of model complexity is that uncertainty in both model structure and parameter estimation increased too. Thus, identification of uncertainty is more and more recognized as an essential part of model application. To quantify how much uncertainty is in the model output (referred to as uncertainty analysis) and where does the uncertainty come from (referred to as sensitivity analysis (SA)) is the goal of every investigation in this field.

Nowadays there are many techniques available which can be used for a SA, i.e. to characterize model input parameters – hereinafter simply referred to as parameters – with respect to their sensitivity. However, there are few methods which do not impose any restriction on the model during its application. Generally, a computational or mathematical model may have non-additive, non-monotone and nonlinear properties. In addition, it may have singularities or regions where the model response is not defined. Finally, parameter correlations may exist. Thus, if we look for a global, model independent method that can be applied to any model owing the properties mentioned above, and if we want to get information not only about the main effects of parameters but also about interaction effects with other parameters, then two methods remain to the authors knowledge: the method of Sobol' and the Fourier Amplitude Sensitivity Test (FAST).

A complete characterization of the sensitivity of model parameters with respect to their main and interaction effects can be done by the calculation of first-order and total sensitivity indices (Saltelli et al. 2012). Unfortunately, total sensitivities cannot be computed with the original FAST method developed long time ago (see e.g. Cukier et al. 1978). Later, Saltelli et al. (1999) published an algorithm known as "Extended FAST" in order to overcome this limitation. Total sensitivity indices can be estimated, however, this method has several disadvantages when investigating models with many, say 30 and more parameters. First, the analysis requires a minimum sample size N that scales with the number of parameters k to be investigated. For example, when using a frequency step width Δ=2, an interference factor M=4, and k=50 we get, according to the Nyquist criterion, a sample size of $N = 1 + 4M^2(1 + (k - 2)\Delta) = 3649$ which is rather high. Further, the model has to be evaluated 3649 times for each parameter to be investigated. Note, that M and Δ cannot be reduced further, otherwise strong interference errors would bias the analysis result. Finally, an accurate estimation of low sensitivity values, approximately below 0.1, is not possible. This is due to the low signal-to-noise ratio of the corresponding Fourier amplitude.

Mara (2009) developed another approach for the calculation of total sensitivity indices using FAST in combination with a random balanced design. In contrast to "Extended FAST", Fourier amplitudes of the complementary frequencies have to be excluded from the Fourier analysis. This means that a lower integration limit j_{min} has to be introduced, in addition to the other operational parameters such as upper integration limit j_{max} = N/2, frequency step width Δ, and non-complementary frequency ω_i. Even if one can find an appropriate parameter set for one model application, the same parameter set may deliver biased results when using it for another model analysis. Generally speaking, the result of the analysis is highly depending on the choice of these four parameters. Moreover, the sample size N should be at least 3000 when using k=30. As with "Extended FAST", the model has to be evaluated N times for each parameter to be investigated. Therefore, this approach as well as "Extended FAST" did not become widely accepted as a general, global sensitivity analysis method.

What remains is the method of Sobol' which is known to be a robust, accurate and model independent approach. Regarding the estimation of total sensitivity indices, different algorithms were proposed by Homma and Saltelli (1996), Sobol (2007), Jansen (1999) and Saltelli (2010), respectively. Though, it is an expensive method in terms of computer runtime because $N(k+1)$ simulations are required to compute all total sensitivity indices. However, it is demonstrated in this article that the cost of this method can be significantly reduced if a bootstrap technique is employed. On the other hand, FAST in combination with random balanced design sampling called RBD-FAST and introduced by Tarantola et al. (2006), is known to be an efficient method for the estimation of main effects, i.e. first-order sensitivity indices. Thus, what would be more logical than to combine RBD-FAST with the Sobol' method? More precisely, the idea is to evaluate the model $N(k+1)$ times in a first step, and then to calculate first-order sensitivity indices using RBD-FAST as well as total sensitivity indices using the Sobol' method in a second step. Further, both methods should use the same set of model evaluations as far as possible. Finally, it should be possible to reuse data of previous model evaluations for a new, more precise sensitivity analysis. It will be shown that this is feasible by means of a shared sampling strategy for both methods based on Sobol's quasi-random sequences. However, the RBD-FAST version by Tarantola et al. has to be modified in order to fulfill these requirements.

The paper is organized as follows. Details of the algorithm and the shared sampling strategy are explained in section 2. The capability and performance of the new method is investigated using an analytical test function, which is described in section 3. Results of the numerical experiment are shown and discussed in section 4. Section 5 provides a summary of this paper.

2 ALGORITHM AND IMPLEMENTATION

2.1 Calculation of Total Sensitivity Indices

The Sobol' method is applied which was further developed by Jansen and Saltelli. In particular, total sensitivity indices are calculated using the estimator by Jansen (1999). As for the sampling strategy, a radial design approach is used together with Sobol's quasi-random numbers (Sobol' 1967) in A-A_B configuration, which was proposed by Saltelli et al. (2010). Quasi-random numbers are sequences of multidimensional points characterized by "optimal" space-filling properties (Saltelli et al. 2012).

However, in order to fulfill the above mentioned requirement of data reuse, the number of rows of matrix A must be always equal to 2^m+1 with m a positive integer. The reason for this restriction is briefly explained using a simple example, i.e. a model with 5 parameters. When applying Sobol's algorithm with m=2, the sequence for the first parameter, i.e. the first dimension, is 0, 0.5, 0.75, 0.25. However, in order to completely explore the parameter space in a uniform manner, 1 is added as first number to that sequence (see the first column of Table 1). In this way, the parameter space is uniformly scanned with a step width of 0.25 (the order of the numbers is not important in this consideration). As for the other parameters (dimensions), the same numbers are applied, however in a different order compared to the first dimension. Matrix A consisting of these 25 numbers can now be used to evaluate the model and to estimate the total sensitivity index for each parameter in a first iteration step. For a next iteration using m=3, the sequence is the same as described above, however with the additional numbers 0.125, 0.375, 0.625, and 0.875. Thus, matrix A contains now 9 numbers in each dimension. It is easily recognized that the space is again uniformly scanned, however with a step width of 0.125. If the first evaluation step was done at an earlier date, then the model needs to be evaluated only four times (using the last four rows) during the second iteration step.

Of course, such low m values are prohibitive in practice since they would yield highly inaccurate results. In this work, $m \geq 7$ was used which yields at least 129 rows. As for the generation of matrix B, the same procedure is applied as suggested by Saltelli et al. (2010). However, since all dimensions of the first three rows of the multi-dimensional sequence contain the same numbers, all numbers of the first, second, and third row of matrix B are replaced by 0.5, 0.5, and 0, respectively, in order to obtain a different matrix B compared to A. As an example of this procedure, the first 9 rows of a 10-dimensional sequence are shown in Table 1. The attentive reader will have noticed that the number of a particular row i and column j in matrix B is not always different to the number at the same location in matrix A, which is a necessary condition to build matrix A_B, e.g. A(9,1) = B(9,1) = 0.125. In this case, the number of one of the following columns within the same row of matrix B is selected for A_B depending on whether the inequality condition is met.

Table 1: First 9 rows of a 10-dimensional quasi-random sequence

Matrix A					**Matrix B**				
1	1	1	1	1	0.5	0.5	0.5	0.5	0.5
0	0	0	0	0	0.5	0.5	0.5	0.5	0.5
0.5	0.5	0.5	0.5	0.5	0	0	0	0	0
0.75	0.25	0.75	0.25	0.75	0.25	0.75	0.25	0.25	0.75
0.25	0.75	0.25	0.75	0.25	0.75	0.25	0.75	0.75	0.25
0.375	0.375	0.625	0.125	0.875	0.875	0.125	0.625	0.125	0.875
0.875	0.875	0.125	0.625	0.375	0.375	0.625	0.125	0.625	0.375
0.625	0.125	0.375	0.375	0.125	0.625	0.875	0.875	0.375	0.125
0.125	0.625	0.875	0.875	0.625	0.125	0.375	0.375	0.875	0.625

The bootstrap technique (see e.g. Efron and Tibshirani 1993) is applied to estimate the uncertainty of the computed total sensitivity indices. This approach relies on resampling with replacement. Basically, a bootstrap sample A^* of size N is created by resampling matrix A with replacement. Then, for each parameter the index is calculated using that model outputs which are solely related to bootstrap sample A^* and the corresponding sample A_B^*. This step is repeated several times to obtain a bootstrap distribution of the index. Finally, the arithmetic mean and 90% confidence interval for each sensitivity index are computed using the underlying distribution.

2.2 Calculation of First-Order Sensitivity Indices

Basically, the algorithm of RBD-FAST introduced by Tarantola et al. (2006) is applied for the calculation of first-order sensitivity indices. The problem of aliasing and interference, as known from the original FAST method, is not an issue when introducing a random balanced design. This means that RBD-FAST does not require a minimum sample size. On the contrary, samples of lower size can be used, even for models with many parameters since a dependency on k does not exist. Computed sensitivity indices are more accurate than indices computed with the original FAST since potential interference effects are absent (Saltelli et al. 2012). Moreover, the method is easy to implement and operate because only the parameters N and M govern the analysis result where M describes the maximum harmonic order to be captured during the Fourier analysis.

Following a shared sampling strategy, the matrix A as described above and employed for the calculation of total sensitivity indices is also used for the calculation of first-order sensitivity indices. This ensures the possibility of reusing data from previous analysis runs. This means on the other hand that sampling is now initiated in the parameter domain in contrast to the other FAST methods where sampling is initiated in the frequency domain and θ-space, respectively (Xu et al. 2011). The consequence is that the corresponding sampling in the frequency domain has to be limited to the range from $-\pi/2$ to $+\pi/2$. In this way, a unique relation between x_i in the parameter domain and the corresponding parameter θ_i in the frequency domain is guaranteed. In particular, is well known that FAST uses a periodic search function $x_i = G(sin\theta_i)$ to explore the parameter domain. For example, Saltelli et al. (1999) proposed the function $x_i = 0.5 + (\arcsin(sin\theta_i))/\pi$ where the frequency depending variable θ_i is uniformly distributed between $-\pi$ and $+\pi$. Note that the independent variable is θ_i and the dependent one x_i. This equation can be solved for θ_i as follows

$$\theta_i = \pi(x_i - 0.5) \qquad i = 1, \dots, k$$

where x_i is now the independent variable uniformly distributed between 0 and 1. Thus, θ_i is uniformly distributed between $-\pi/2$ and $+\pi/2$. The consequence is that the Fourier analysis has to be performed in the range $-\pi/2 \dots + \pi/2$. This is possible without any limitation by utilizing the symmetry properties of FAST (Cukier et al. 1978, Koda et al. 1979). In this way, the integration range is reduced by one half, and therefore also the number of required model evaluations (Koda et al. 1979). In the following, the equations proposed by Koda et al. are used during the Fourier analysis. It should be emphasized that sampling in the parameter domain has to be uniform in the range 0…1 when applying our approach. Therefore, the matrices A_B as generated for the Sobol' analysis cannot be used for RBD-FAST because their sampling properties are partly nonuniform.

To reduce the effect of sampling errors on the analysis result, a statistical Z-test is applied to select only those Fourier coefficients which are significantly larger or smaller than zero. The procedure as suggested by Xu et al. (2011) is applied, therefore the interested reader is referred to the corresponding reference for more details.

2.3 Implementation

Below a summary of the overall procedure is provided in order to better illustrate the analysis method. The steps are as follows:

(1) Generate a matrix of quasi-random numbers consisting of $N = 2^m$+1 rows and $2k$ columns.
(2) Define matrices A and B as well as for each parameter x_i the matrix A_B^i considering the modifications described above.
(3) For each row of matrix A and A_B^i compute real model parameters considering the numbers of each row as normalized parameters, and run the model using this parameter set.
(4) Compute the total sensitivity index S_{T_i} for each parameter x_i using the estimator by Jansen. Then, create a batch of bootstrap samples A^* by resampling matrix A with replacement. Generate boots-

trap distributions by computing the index $S^b_{T_{i,j}}$ for each bootstrap sample j. Calculate the mean and 90% confidence interval for each index using the underlying distribution.

(5) As part of RBD-FAST, re-order the model outputs as obtained from matrix A with respect to the order of the corresponding parameter x_i. Then, compute the Fourier coefficients using the equations for the symmetrical case. Apply a Z-test to select only those Fourier coefficients which are significantly larger or smaller than zero. Finally, compute first-order sensitivity indices using the selected coefficients.

It should be noted that step (4) can be done concurrently to step (5) since dependencies between these steps do not exist.

3 NUMERICAL EXPERIMENTS

3.1 Methodology

A series of computer experiments using an analytical test function was carried out in order to evaluate the method described above. The test function applied is presented in the next section. As for the sampling, m = 7, 8, …, 14 was used to create base samples of increasing size N, i.e. matrices A with 129, 257, …, 16385 rows. As for the main effects, first-order sensitivity indices were calculated without applying the Z-test. For comparison, the indices were re-calculated in a second run, however with applying the Z-test using a significance level of 0.01. In all cases, Fourier coefficients up to the 10th harmonic order were considered (M=10). Finally, total sensitivity indices were calculated with and without applying the bootstrap technique. For each parameter, a bootstrap distribution was generated by computing total sensitivity indices from 10000 bootstrap samples. These distributions were then employed to calculate means and 90% confidence intervals for the total sensitivities.

3.2 Test Function

The method described in section 2 was tested on an analytical test function commonly used as benchmark in SA. In particular, the G-function by Sobol (see e.g. Saltelli et al. 2010) was applied

$$G = \prod_{i=1}^{k} \frac{|4x_i - 2| + a_i}{1 + a_i}$$

with k=30, the constants $a_i \in \mathbb{R}^+$, and the parameters x_i being uniformly distributed in [0,1]. The value of a particular a_i determines the relative importance of x_i, i.e. the smaller a_i the more important x_i. For a first test case, the constants a_i were set as follows: a_1 = 0, a_2 = 1, a_3 = 2, a_4 = 19, and 99 for all other a_i. Thus, x_1 exhibits the highest sensitivity followed by the other parameters with increasing index i. Sensitivity indices, which can be computed analytically for this function (Saltelli et al. 2010), are given in Table 2.

Table 2: First-order and total sensitivity indices calculated for test case 1

i	a_i	S_i	S_{Ti}
1	0	0.666013	0.749510
2	1	0.166503	0.230618
3	2	0.074001	0.107073
4	19	0.001665	0.002496
5…30	99	0.000067	0.000100

For a second test case, the constants a_1, a_2, a_3, a_4, and a_5 were set to zero and all other a_i to 99. Thus, the first five parameters have the same sensitivity which is significantly higher than the one of the remaining parameters. Analytical computed sensitivity indices for both parameter groups are given in Table 3.

Table 3: First-order and total sensitivity indices calculated for test case 2

i	a_i	S_i	S_{Ti}
1…5	0	0.103600	0.327700
6…30	99	0.000010	0.000044

4 RESULTS AND DISCUSSION

First-order and total sensitivity indices were calculated for the test case 1 applying the method described above. The result obtained for parameter x_1 is illustrated as a function of iteration in Figure 1. As for the first iteration, a base sample (matrix A) with 129 rows was used. For each of the following iteration steps, the sample size is roughly doubled with increasing iteration number, i.e. N = 257, 513, …, 16385 at the iteration step 2, 3, …, 8. The analytic value of the sensitivity index is represented by a solid line whereas a 10% deviation from this value is represented by a dashed line.

Clearly, sensitivities converge to their analytic values with increasing iteration number. As for the first-order sensitivity index, the Z-test does not seem to improve the accuracy of the calculated index which can however be expected because the Z-test should not impact the result of the most influential parameters. This is due to the fact that usually all Fourier coefficients are statistically significant and therefore selected during the test, which was observed from the second iteration onwards in this example.

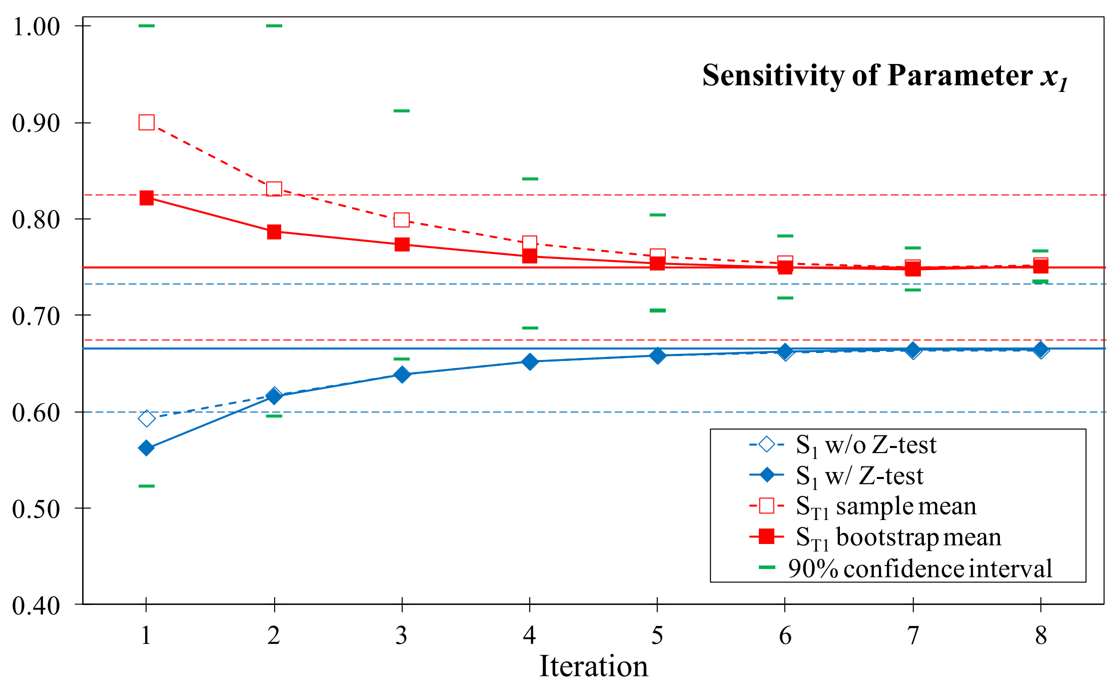

Figure 1: Results for parameter x_1 as computed with/without applying the Z-test and with/without applying the bootstrap technique, respectively.

As for the total sensitivity index, there is a noticeable difference between the sample mean and the bootstrap mean, especially at the first and second iteration, which becomes smaller with increasing sample size. This is not surprising because the Sobol' method is known to be inaccurate at small sample sizes. On the other hand, it is also known that the bootstrap technique offers advantages in terms of ranking of sensitivity indices (Yang 2011). Thus, the bootstrap method may significantly improve the accuracy of the computed index as can be seen in Figure 1. Note that after the second iteration S_1 and the bootstrap mean of S_{T1} are already within a 10% error range, S_{T1} even after the first iteration. Nevertheless, the confidence interval as calculated for the total sensitivity index is large at small sample size but decrease steadily with each subsequent iteration.

As can be seen in Figure 2 and 3, respectively, the sensitivities of the parameters x_2 and x_3 also converge to their analytic values. However, first-order sensitivities are strongly overestimated, especially at the first two iterations, if a Z-test is not applied. The reason for this observation is simply the fact that all Fourier coefficients, especially those which are not statistically significant, are considered during the analysis. On the other hand, the Z-test significantly improves the accuracy in the determination of the first-order sensitivities. Also, the bootstrap technique helps a lot to improve the estimates for the total sensitivity index as in the case of parameter x_1.

This also holds for the remaining parameters x_4 ... x_{30} which were correctly classified as non-influential parameters due to their low sensitivity. However, to illustrate the effect of the Z-test for a non-influential parameter, results are shown for parameter x_4. As can be seen in Figure 4, S_4 is far beyond its analytic value and even larger than S_{T4} at the first four iterations if the Z-test is not applied. On the other hand, at the first five iterations the application of the test leads to an exclusion of all Fourier coefficients from the index calculation because they are too small to be considered. Thus, $S_4 = 0$ is obtained. Only from the 6^{th} iteration onwards Fourier coefficients are partly detected as statistically significant and thus contributing to S_4.

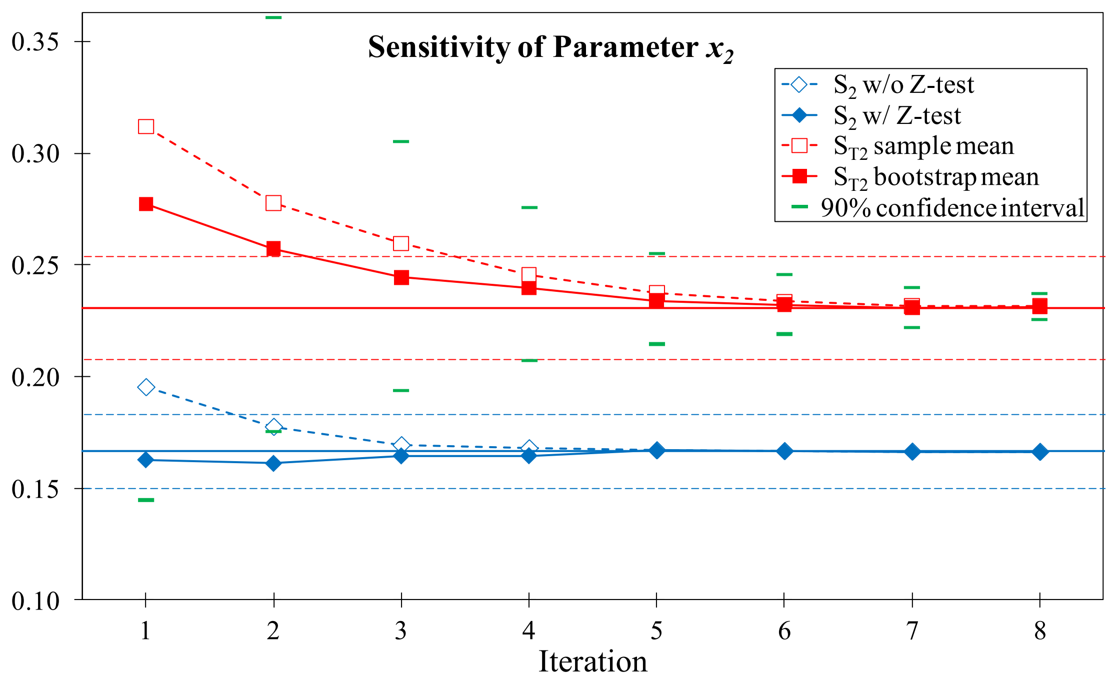

Figure 2: Results for parameter x_2 as computed with/without applying the Z-test and with/without applying the bootstrap technique, respectively.

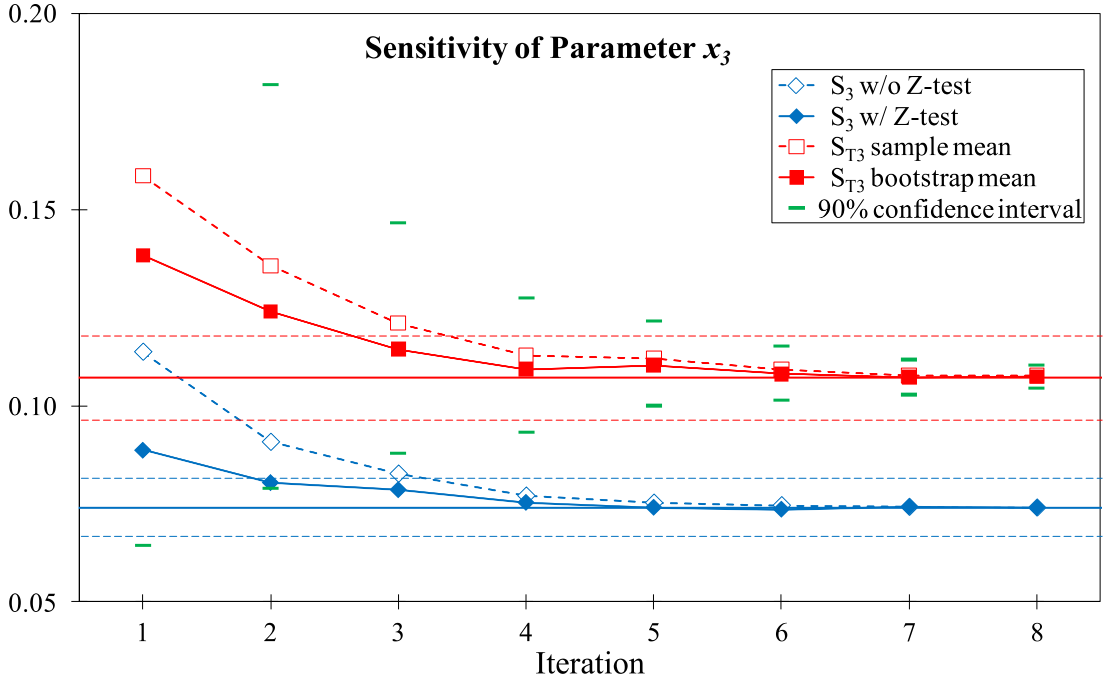

Figure 3: Results for parameter x_3 as computed with/without applying the Z-test and with/without applying the bootstrap technique, respectively.

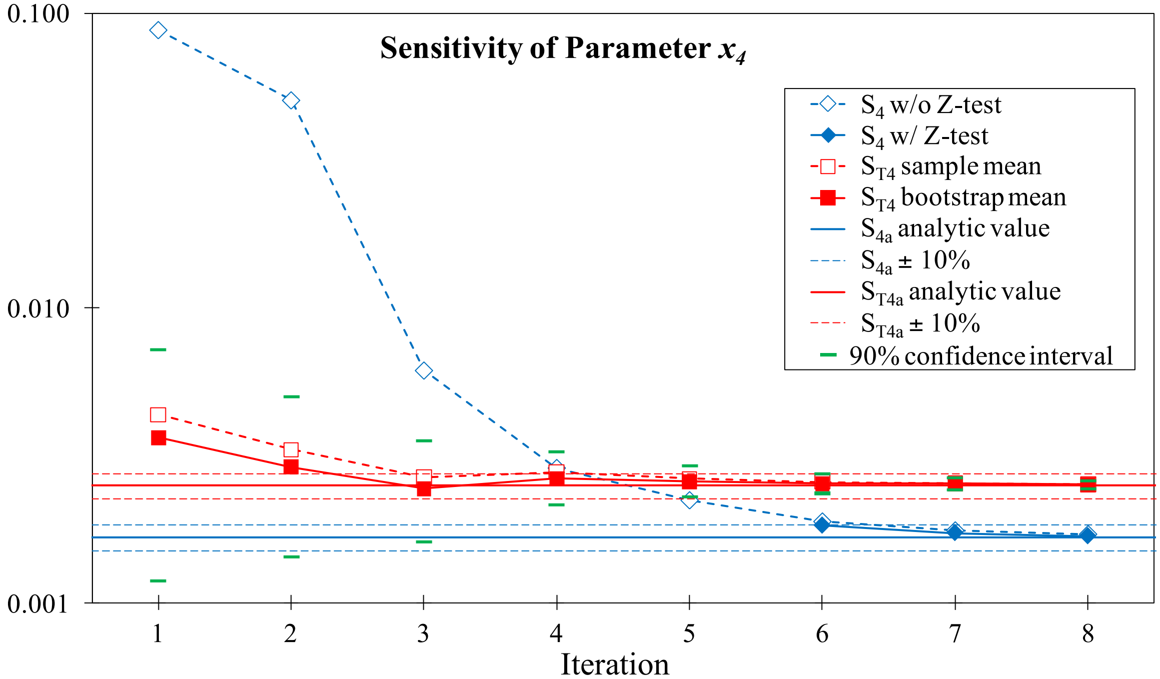

Figure 4: Results for parameter x_4 as computed with/without applying the Z-test and with/without applying the bootstrap technique, respectively.

Hence, a large sample size would be required to characterize the main effect of a non-sensitive parameter with sufficient precision. However, this is not our goal since we are interested in getting a parameter ranking. In the case of independent parameters, the total sensitivity index provides a reliable measure for the parameter ranking of importance. Therefore, all we need to do is just draw all total indices together with their confidence intervals in one plot and analyze whether any two intervals overlap. Figure 5 illustrates that intervals of the total sensitivities partly overlap at the first iteration, however, no more overlap is apparent from the second iteration onwards. Thus, definite conclusions in terms of importance ranking are already obtained at the second iteration step, i.e. the parameter with the highest sensitivity index (S_{T1}) outranks the others, the parameter with the second highest index (S_{T2}) outranks the others except the first parameter and so on. As expected, the final parameter ranking obtained is identical to the ranking based on the analytical indices.

Information about the main effects of model parameters can be gained from first-order sensitivity indices that can also be calculated using the Sobol' method. In order to compare the convergence behavior between the Sobol' method and our approach, first-order indices were recalculated using the estimator of Saltelli et al. (2010) and the generated matrices B and A_B^i. The result is exemplary shown for parameter x_1 (see Figure 6). Clearly, the index S_1 computed by RBD-FAST converges faster to the analytic value than the one computed by the Sobol' method. This behavior was observed for all parameters. In fact, it is generally known that FAST is superior in terms of convergence compared to the Sobol' method (see e.g. Gatelli et al. 2009). It should be noted that the exclusive use of the Sobol' method for the calculation of first-order and total sensitivity indices requires N additional model evaluations compared to our approach. In other words, information about the main effects is obtained at no extra computational cost when applying our method.

As a final note to the application of the bootstrap technique, this method cannot be employed in RBD-FAST for the following reason. A resampling of the base sample would result in a nonuniform and nonperiodic sampling in the frequency domain, which distorts the periodic signal RBD-FAST is relied on. Thus, unreliable estimates of bootstrap means and confidence intervals would be obtained.

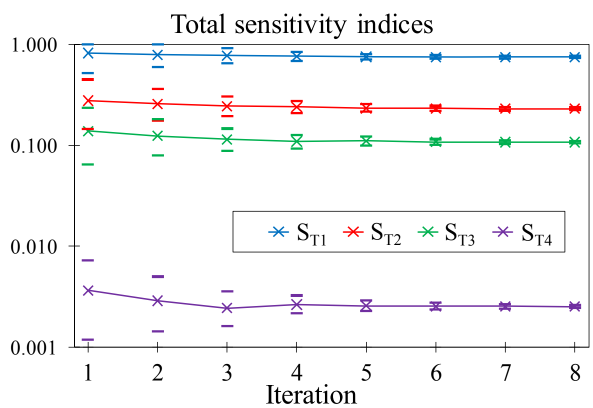

Figure 5: Total sensitivity indices as calculated for the first four parameters.

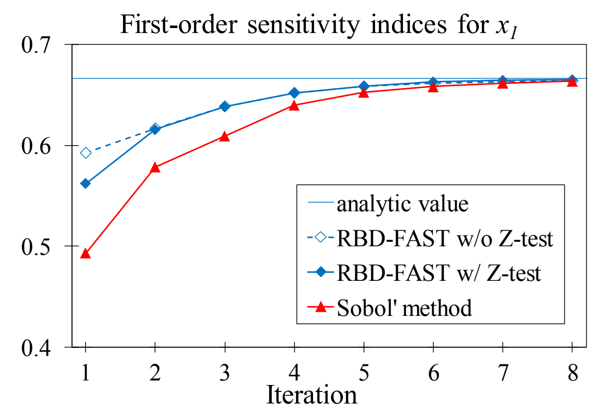

Figure 6: First-order sensitivities for x_1 calculated with RBD-FAST and the Sobol' method, respect.

As for test case 2, the results obtained for each parameter of the first group were very similar, therefore mean sensitivities averaged over these five parameters are briefly discussed here. As for the total sensitivity, the bootstrap technique also improves the estimate for this index in this case (see Figure 7). Remarkable is that the index converges much more slowly to its analytic value compared to test case 1. Obviously, this is a very difficult test case, as also previously stated by other authors (see e.g. Saltelli and Sobol 1995), where strong interactions between parameters occur. As expected for parameters of high importance, first-order sensitivities calculated with applying the Z-test differ very little from those calculated without applying the test.

As a final remark, our approach has also been evaluated using other test functions (not shown here). Overall, the bootstrap technique and the Z-test improves the algorithm presented above. Moreover, the

RBD-FAST algorithm has been successfully tested on models with correlated parameters applying the "restricted pairing technique" of Iman and Conover (Iman and Conover 1982). Thus, parameter correlations can be considered during the analysis of main effects. Unfortunately, this technique cannot applied during the calculation of total sensitivities as described above because the variance decomposition as proposed by Sobol' and used in our approach requires fully independent parameters (Saltelli 2002).

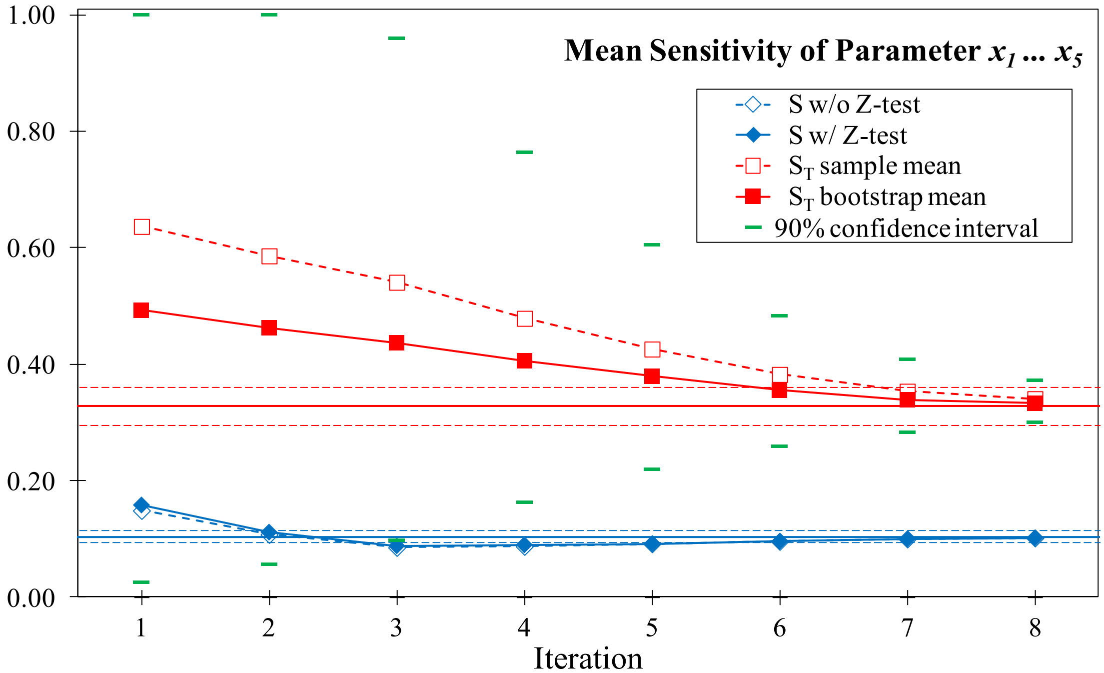

Figure 7: Results of the second test case as computed with/without applying the Z-test and with/without applying the bootstrap technique, respectively.

CONCLUSIONS

For the first time, two complementing variance-based methods, the Sobol'-method and RBD-FAST, were combined for a global sensitivity analysis of a nonlinear mathematical model. A combination of these two methods is feasible if a shared sampling strategy is used. In particular, the method suggests the generation of a base sample by applying a radial design approach together with Sobol's quasi-random sequences. Then, total sensitivity indices can be estimated using the Sobol'-Saltelli method whereas first-order sensitivity indices can be concurrently computed using a modified version of RBD-FAST. The feasibility and capability of the method was investigated using an analytical test function commonly used as benchmark in the field of sensitivity analysis. It was shown that the method can be used for a global sensitivity analysis of a nonlinear model without assuming any restrictions on the model except that model input parameters have to be independent and uniformly distributed. However, correlations between parameters can be considered in the course of the analysis of main effects if the given correlation structure is preserved by applying e.g. the method of Iman and Conover (Iman and Conover 1982).

The bootstrap technique was applied to evaluate the uncertainty of the calculated total sensitivity indices by the computation of confidence bounds. Further, the bootstrap means of the indices help to improve the accuracy of the method in terms of parameter ranking. Moreover, information about the main effects of model parameters, i.e. first-order sensitivity indices were obtained at no extra computational cost. The accuracy in the determination of these indices can be improved by applying a statistical Z-test. Last but no least, data of previous model evaluations can be reused for a new, more precise sensitivity analysis. However, as a trade-off the size of the base sample has to be doubled in this case.

The approach developed is part of our framework consisting of software tools for screening, sensitivity analysis and optimization of model parameters. In particular, it makes sense to do a screening analysis if the model has many parameters and/or is computationally expensive to evaluate, as in the case of hydrogeological models. It is known that such models need a parameter calibration which can be done using a three-step procedure. The first step would be a screening analysis which allows a classification of parameters into important and non-important ones. For this purpose, an efficient screening algorithm was developed recently (Henkel et al. 2011). In a second step, the important parameters are analyzed in more detail using the approach described above. The third step would be the optimization of parameters ranked as important, which can be done by using e.g. our optimization software ISSOP® (Krug 2002).

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