

Investigation of determinism-related issues in the Sobol' low-discrepancy sequence for producing sound global sensitivity analysis indices

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Abstract

A computationally efficient and robust sampling scheme can support a sensitivity analysis of models to discover their behaviour through Quasi Monte Carlo approximation. This is especially useful for complex models, as often occur in environmental domains when model runtime can be prohibitive. The Sobol' sequence is one of the most used quasi-random low-discrepancy sequences as it can explore the parameter space significantly more evenly than pseudo-random sequences. The built-in determinism of the Sobol' sequence assists in achieving this

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attractive property. However, the Sobol' sequence tends to deteriorate in the sense that the estimated errors are distributed inconsistently across model parameters as the dimensions of a model increase. By testing multiple Sobol' sequence implementations, it is clear that the deterministic nature of the Sobol' sequence occasionally introduces relatively large errors in sensitivity indices produced by well-known global sensitivity analysis methods, and that the errors do not diminish by averaging through multiple replications. Problematic sensitivity indices may mistakenly guide modellers to make type I and II errors in trying to identify sensitive parameters, and this will potentially impact model reduction attempts based on these sensitivity measurements. This work investigates the cause of the Sobol' sequence's determinism-related issues.

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1 Introduction

With the development of computer power, modellers and researchers largely rely on building models to mimic, understand and predict aspects of natural phenomena and increasingly their links with human actions. But the models have become much more complicated and difficult to interrogate and analyse.

Global sensitivity analysis (GSA) methods have received significant attention over recent years as they have the capability for reducing model complexity and understanding model behaviour. However, GSA methods rely on the selected strategy used to sample model factors (parameters and model inputs) to generate the model response surface from which sensitivity indices are calculated. As each sample of factors leads to a forward model simulation, a sampling scheme may need to be efficient in line with the computational budget, especially where model runtimes are prohibitive. But any efficient sampling scheme must also provide SA measures with the desired properties, such as acceptable convergence rates. It is common to study the impact of sampling strategies by using benchmark testing functions, as is done by Tarantola et al. [8].

Tarantola et al. [8] compared the Sobol' sequence and Latin Supercube sampling methods under the Sobol' variance-based sensitivity analysis method, and concluded that the Sobol' sequence is better and appropriate under most circumstances. The Sobol' variance-based sensitivity analysis method and the Sobol' sequence are discussed in more detail in Section 2. The results shown by Tarantola et al. indicated that the Sobol' sequence may occasionally experience large errors for one or multiple input index values [8, bottom right of Figure 9], but they simply explained this error spike as a deterioration of the Sobol' sequence under high dimensions. The error spike is recognised as the index value of one or more factors having particularly large errors compared to the index values of other factors. It is worth noting that this error spike issue may not easily be identified for practical problems where model inputs tend to have different sensitivities. For the case in Figure 1, the error spike is observed because all input variables have the same expected sensitivity; however, modellers or end users may find it difficult to identify if certain inputs have incorrect index values for actual model applications. Thus, it is of utmost importance to investigate the cause of this error spike.

Randomized Sobol' sequences such as the scramble method, random shift method, and newly developed column shift method [7] effectively avoid the determinism issues of the original Sobol' points. For this article, we

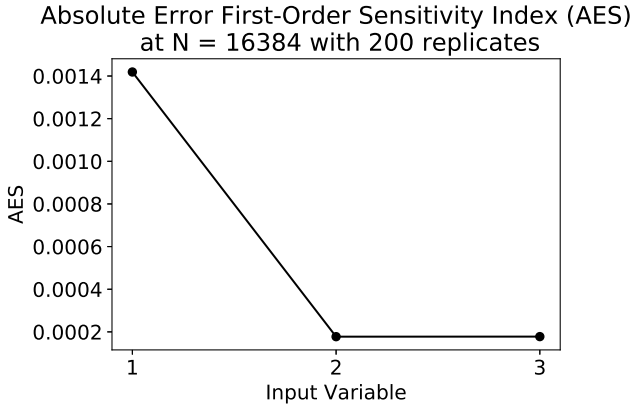


Figure 1: The first-order sensitivity indices of the Sobol' sequence for a multi-linear function, where the input 1 has much higher error than other inputs.

focus on investigating the determinism-related issues of the original Sobol' sequences without the aid of randomization methods. By recreating the same experiments in Tarantola et al. [8], we find the same error spikes even at relatively low dimensions. In addition, we find that the error spikes do not diminish by averaging the errors across multiple replications, and the inner determinism of the Sobol' sequence may cause the error spike. To investigate this error spike, we propose a simple multi-linear function to test and explore its causes in more details in Section 3.

2 Experiment set-up

2.1 Sobol' variance-based method

In this subsection, we briefly overview the Sobol' variance-based method [11], which is one of the most popular global SA methods due to its model independence, ease of use, and ability to evaluate how changes in factors affect model output variance, both with and without interactions. Given a

square-integrable function

$$Y = f(\mathbf{X}) = f(X_1, \dots, X_p),$$

where $\mathbf{X} = (X_1, \dots, X_p)$ is a vector of p model parameters, Y is a scalar model output and function f is defined over a p -dimensional unit hypercube

$$\Omega = (\mathbf{X} \mid 0 \leq x_i \leq 1; i = 1, \dots, p).$$

Assuming that the input variables \mathbf{X} are all independent, the model output variance $V(Y)$ is decomposed as

$$V(Y) = \sum_{i=1}^p V_i + \left(\sum_{i=1}^{p-1} \sum_{j=i+1}^p V_{ij} \right) + \dots + V_{1,\dots,p},$$

where $V_i = V(f_i(X_i))$ and $V_{ij} = V(f_{ij}(X_i, X_j))$ are the corresponding partial variances, and similarly $V_{1,\dots,p} = V(f_{1,\dots,p}(X_1, \dots, X_p))$. The first-order sensitivity index S_i of an individual input is obtained by dividing the first term of the decomposition V_i by the model output variance $V(Y)$:

$$S_i = \frac{V_i}{V(Y)} \approx \frac{\frac{1}{N} \sum_{j=1}^N f(\mathbf{B})_j [f(\mathbf{A}_B^{(i)})_j - f(\mathbf{A})_j]}{V(Y)}. \quad (1)$$

where N is the number of samples. To estimate the sensitivity indices using Monte Carlo integrals, an $N \times 2p$ sample matrix is generated through the Sobol' sequence for each experiment giving sample matrices \mathbf{A} and \mathbf{B} ; see Figure 2. Matrices \mathbf{A} and \mathbf{B} are used in the approximations in equation (1), and $\mathbf{A}_B^{(i)}$ is a sample matrix created by replacing the i th column of matrix \mathbf{A} with the i th column of matrix \mathbf{B} but keeping the rest of the matrix the same.

To evaluate the performance of selected sampling strategies, Tarantola et al. [8] used the absolute error across R different replicates. The absolute error for the first-order sensitivity index (AES) is:

$$AES = \frac{1}{R} \sum_{r=1}^R |S_i^{(r)} - \hat{S}_i|, \quad (2)$$

where $S_i^{(r)}$ is the estimated S_i of the r th replicate, and \hat{S}_i is the analytical S_i .

$$\mathbf{N} \begin{bmatrix} \mathbf{A} & \text{---} & \mathbf{B} \end{bmatrix} \begin{matrix} 2\mathbf{p} \\ \mathbf{p} \end{matrix}$$

Figure 2: Generated $\mathbf{N} \times 2\mathbf{p}$ sample matrix from the Sobol' sequence. Sample matrix \mathbf{A} is the left $\mathbf{N} \times \mathbf{p}$ matrix, and the sample matrix \mathbf{B} is the right $\mathbf{N} \times \mathbf{p}$ matrix.

2.2 Sobol' quasi-Monte Carlo sequence

The Sobol' low-discrepancy sequence was initially proposed by Sobol' [10], and it is one of a number of quasi-Monte Carlo sampling strategies that generate structured samples compared to the basic pseudo-random Monte Carlo sequence. To generate the i th dimension of the j th Sobol' point $x_{j,i}$, the Sobol' sequence uses a group of direction numbers $v_{1,i}, v_{2,i}, \dots, v_{d_i,i}$ and a primitive polynomial of degree d_i in the field \mathbb{Z}_2 :

$$x^{d_i} + a_{1,i}x^{d_i-1} + a_{2,i}x^{d_i-2} + \dots + a_{d_i-1,i}x + 1,$$

where the coefficients $a_{1,i}, \dots, a_{d_i-1,i} = 0$ or 1 . These coefficients are used to define a sequence of positive integers by the recurrence relation

$$m_s = 2a_{1,i}m_{s-1,i} \oplus 2^2a_{2,i}m_{s-2,i} \oplus \dots \oplus 2^{d_i-1}a_{d_i-1,i}m_{s-d_i+1,i} \oplus 2^{d_i}m_{s-d_i,i} \oplus m_{s-d_i,i},$$

for $s \geq d_i + 1$, and \oplus is the bit-wise XOR operator. The values of $m_{s,i}$ for $s \leq d_i$ are freely chosen but with the restriction of being odd integers and less than 2^s . Assuming two integers where $y \geq z$, the mathematical equivalent of the bit-wise XOR operator is

$$y \oplus z = \sum_{n=0}^{\lfloor \log_2(y) \rfloor} 2^n \left[\left(\left\lfloor \frac{y}{2^n} \right\rfloor + \left\lfloor \frac{z}{2^n} \right\rfloor \right) \bmod 2 \right]. \tag{3}$$

The group of direction numbers $v_{1,i}, v_{2,i}, \dots, v_{d_i,i}$ is then defined as

$$v_{s,i} = \frac{m_{s,i}}{2^s}.$$

Then the Sobol' point of interest is defined as

$$x_{j,i} = \mathbf{b}_1 v_{1,i} \oplus \mathbf{b}_2 v_{2,i} \oplus \cdots \oplus \mathbf{b}_h v_{h,i},$$

where \mathbf{b}_l is the l th bit from the right of number j in binary, for example $(j)_2 = \mathbf{b}_h \cdots \mathbf{b}_2 \mathbf{b}_1$. Antonov and Saleev [1] proposed the use of grey code $(j)_2 = \mathbf{g}_h \cdots \mathbf{g}_2 \mathbf{g}_1$ instead of binary code $(\mathbf{b}_h \cdots \mathbf{b}_2 \mathbf{b}_1)$ to increase the computational efficiency. Grey code only changes one bit from one number in binary to the next consecutive one in binary, and it does not affect the asymptotic discrepancy of the original Sobol' sequence. This article uses the Sobol' sequence generator code and the $30 \times \mathbf{p}$ direction number matrix \mathcal{V} provided by the Chaospy python library [3], where $\mathbf{p} < 40$ is the number of dimensions limited to the maximum size of arrays set provided by the direction number matrix

$$\mathcal{V} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_{30} \end{bmatrix} = \begin{bmatrix} v_{1,1} & \cdots & v_{1,i} & \cdots & v_{1,p} \\ v_{2,1} & & \cdots & & v_{2,p} \\ \vdots & & & & \vdots \\ v_{30,1} & \cdots & & & v_{30,p} \end{bmatrix}. \quad (4)$$

Bratley and Fox [2] and Joe and Kuo [5] give the above definitions for generating the Sobol' sequence and further details, whilst the definition of discrepancy is given by Tezuka [9].

2.3 Multi-linear function

We propose a simple multi-linear function with the same multi-linear characteristic as the benchmark testing function employed by Tarantola et al. [8]:

$$Y = f(\mathbf{X}) = X_1 \times X_2 \times \cdots \times X_p,$$

where \mathbf{p} is the number of dimensions. We choose $\mathbf{p} = 3$, and the function Y is now defined over a three-dimensional unit hypercube Ω . In theory, the sensitivity indices S_i of model inputs for this multi-linear function are identical. We generate the sample matrix with $2\mathbf{p}$ dimensions and as indicated in Figure 2, the size of the direction number matrix \mathcal{V} is 30×6 .

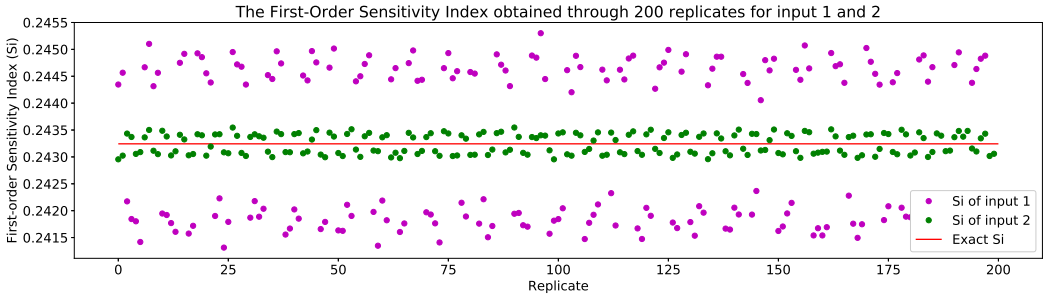


Figure 3: The x-axis indicates which replicate is used, where each replicate comprises the results obtained from an independent experiment, and the y-axis shows the value of the first-order sensitivity index. The 200 magenta and green dots indicate the index values of input 1 and input 2 corresponding to 200 replicates, and the red horizontal line shows the exact analytical index value.

3 Understanding the problem

Morokoff and Caffisch [6] proposed the idea of filling-in-holes to explain potentially poor dimension pairing and correlation issues in the Sobol' sequence, as 16384 samples are needed to achieve almost perfect uniformity for the two-dimensional projection plots of the Sobol' sequence. Following Morokoff and Caffisch, and to largely explore the parameter space, we decided to use 16384 samples, but with 200 different replicates for our experiments. The results in terms of AES for the first-order sensitivity indices of the three-dimensional multi-linear function at $N = 16384$ samples, averaged through 200 replicates, is shown in Figure 1. The AES of input 1 produces observably larger error than both inputs 2 and 3. We pulled out the first-order sensitivity indices of inputs 1 and 2, which have the most distinct behaviour in their relative absolute error, and compared them by drawing a scatter plot of 200 replicates in Figure 3.

It is interesting to see that the index values of input 2 in green are all scattered quite close to the line of the exact S_i , but the index values of input 1 in

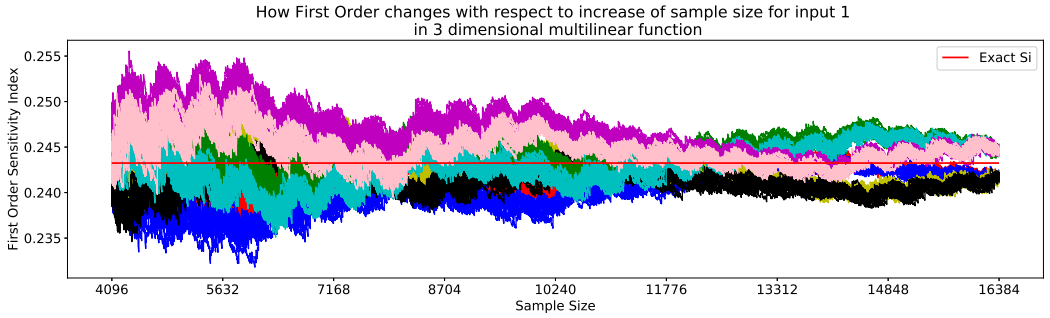


Figure 4: The x -axis indicates the number of samples from 4096 to 16384, and the y -axis shows the value of the first-order sensitivity index. The red horizontal line is the exact first-order S_i for input 1 of the three-dimensional multi-linear function. This plot consists of results from 200 replicates, and eight different groups of replicates are plotted in different colours to indicate distinct oscillation patterns.

magenta are all scattered a certain distance away from the exact S_i line and the green dots. Recall that the calculation of the absolute error in equation (2) measures the average distance of each estimated index value to the analytical value. In our test case, every estimated index value of input 1 is much further away from the analytical value than those of input 2, thus the absolute error of input 1 is much higher than input 2 and resolves the error spike. By inspecting the error spikes of the total-effect sensitivity index, we made similar observations. The use of absolute error, along with relative absolute error, can be problematic under this case, and an alternative performance metric should be considered to avoid the error spike issue; for example, averaging the index values across replicates first then finding the difference from the analytical value \hat{S}_i . However, one may not be able to employ replication due to a limited budget, and this would result in only a single or a small number of model runs, which would then require investigation on the the unusual structure of input 1 in order to avoid the error spike.

By inspecting the changes in S_i with respect to the number of samples, we

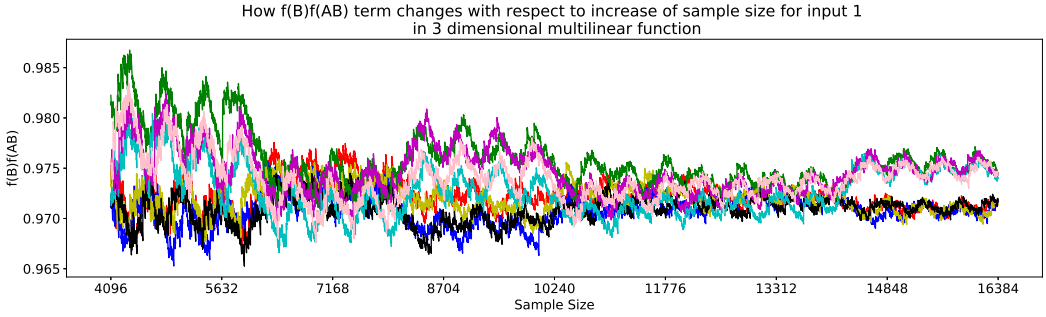


Figure 5: The x -axis indicates the number of samples from 4096 to 16384, and the y -axis shows equation (6) for input 1, and this term is a component of equation (1). This plot consists of results from one replicate from each group, and the eight different replicates are colour coded the same as Figure 4.

conclude that the structure observed in Figure 3 is not stationary. In fact, the behaviour of S_i for input 1 follows a structured oscillation pattern, as indicated in Figure 4, and the first-order index values for inputs 2 and 3 all follow a similar oscillation pattern with the change in the number of samples.

Recall that equation (1) for approximating the first-order sensitivity index S_i consists of two different terms: $f(B)f(A)$ represented as

$$\sum_{j=1}^N \frac{f(B)_j f(A)_j}{NV(Y)}; \tag{5}$$

and $f(B)f(AB)$ represented as

$$\sum_{j=1}^N \frac{f(B)_j f(A_B^{(i)})_j}{NV(Y)}, \tag{6}$$

for convenience. The values of the second term for input 1 with respect to the number of samples is seen in Figure 5. The error spike of input 1 at $N = 16384$ is caused specifically by the noticeable separation of the higher

pink group of replicates and the lower black group of replicates in Figure 5. There are eight general patterns within the total 200 replicates, as indicated by eight different colours in Figure 4, and Figure 5 shows one replicate from each pattern group.

4 Discussion and conclusions

The generation of Sobol' points strictly follows the direction matrix \mathcal{V} in equation (4), and the first seven points of the Sobol' sequence are calculated through

$$\begin{aligned} \mathbf{x}_1 &= \mathbf{v}_0, & \mathbf{x}_2 &= \mathbf{v}_0 \oplus \mathbf{v}_1, & \mathbf{x}_3 &= \mathbf{v}_1, & \mathbf{x}_4 &= \mathbf{v}_1 \oplus \mathbf{v}_2, \\ \mathbf{x}_5 &= \mathbf{v}_0 \oplus \mathbf{v}_1 \oplus \mathbf{v}_2, & \mathbf{x}_6 &= \mathbf{v}_0 \oplus \mathbf{v}_2, & \mathbf{x}_7 &= \mathbf{v}_2. \end{aligned}$$

Following this order, \mathbf{x}_8 is obtained through $\mathbf{v}_2 \oplus \mathbf{v}_3$, and \mathbf{x}_9 will be $\mathbf{v}_0 \oplus \mathbf{v}_2 \oplus \mathbf{v}_3$. Therefore, there are 2^k points obtained through the combination of $\mathbf{v}_0, \mathbf{v}_1, \dots, \mathbf{v}_k$ joined by the bit-wise XOR operator. These new 2^k points are constructed by joining the previous 2^{k-1} points in reverse order with \mathbf{v}_k , and the last new point is just \mathbf{v}_k .

The second replicate (shown as a cyan colour line in Figure 5) consists of the 16384th to the 32767th Sobol' point, and these 16384 points are obtained through $\mathbf{v}_0, \mathbf{v}_1, \dots, \mathbf{v}_{14}$ but with the Sobol' point $(\mathbf{v}_{14} \oplus \mathbf{v}_{15})$ instead of $(\mathbf{v}_{13} \oplus \mathbf{v}_{14})$. The third replicate (shown as a blue colour line in Figure 5) consists of 16384 Sobol' points constructed from a bit-wise XOR of every single point in the second replicate with \mathbf{v}_{15} except for the 32768th point ($= \mathbf{v}_{14} \oplus \mathbf{v}_{15}$). The six direction numbers $\mathbf{v}_{15,1}, \dots, \mathbf{v}_{15,6}$ in vector \mathbf{v}_{15} can cause very limited changes and still retain the strong correlation pattern as from the second replicate, and this applies to the remaining replicates as well.

The correlation relationship in the direction number matrix \mathcal{V} highly affects the calculations of the variance-based sensitivity analysis, and this determinism is amplified through the use of the absolute error performance metric. For future study, we aim to mathematically formulate the exact upper bound and lower

bound of the first-order sensitivity index S_i for specific numbers of samples with the provided direction number matrix \mathcal{V} for a simple linear function. Then, based on the results of the linear function, we intend to branch out to more types of functions. In addition, a more advanced direction number matrix has been developed, with up to 21 201 dimensions [4] rather than 40 dimensions. The change of direction number causing different sensitivity index behaviour is also worth investigating. By controlling the correlation impact of different direction numbers for models with certain characteristics, one can greatly increase the efficiency of utilising the Sobol' sequence in particular, and the reliability of variance-based sensitivity analysis in general.

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