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Optimising the convergence of a Sobol’ sensitivity analysis for an environmental model: application of an appropriate estimate for the square of the expectation value and the total variance

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Abstract: Over-parameterisation is a key issue in (integrated) environmental modelling. Therefore, a sensitivity analysis (SA) can assist in the proper application of a complex environmental model, such as the Soil and Water Assessment Tool (SWAT). A very powerful sensitivity analysis technique that is gaining popularity in environmental modelling is the variance-based Sobol’ method. Still, the high number of model evaluations necessary to perform the analysis is a major restriction for the method’s use and, as a consequence, an optimised convergence is of the utmost importance. Therefore, this paper presents a study of the influence of some computational issues on the convergence of the sensitivity measures of the Sobol’ SA, i.e. the sensitivity indices. The latter indices are assessed by means of Monte Carlo integrals. These numerical integrals are also used for the estimation of the square of the expectation value and the total variance of the model output, which are important for the computation of the sensitivity indices. The paper investigates the impact of the use of different formulas for the calculation of the integrals of these statistics. We will also show that the choice of the calculation method highly affects the convergence of the sensitivity indices. Finally, we will demonstrate that the convergence of the first order sensitivity indices is mainly determined by the formula used for the estimation of the square of the expectation value, while the convergence of the total sensitivity indices is mainly affected by the equation used for the estimation of the total variance.

Keywords: Sensitivity analysis; Sobol’ method; Convergence; Monte Carlo Integrals; SWAT.

1 INTRODUCTION

Due to a better knowledge of the environmental processes and the general increase of the computational capacity, environmental models have often become more complex over the past decade(s). The representation of the processes in these models is controlled by a high number of parameters. The latter restricts the application of complex environmental models, as an accurate estimation of the values of all the parameters is almost impossible, since the parameter estimation process turns out to be a high-dimensional and mainly non-linear problem. As a consequence, over-parameterisation has become a key issue in (integrated) environmental modelling [Beven, 2000; Saltelli et al., 2006].
A possible strategy to handle over-parameterisation is to perform a sensitivity analysis (SA). This allows to determine the most influential and non-influential parameters of a model and hence to reduce the number of parameters included in the parameter estimation by applying factor fixing (FF), i.e. the process of setting non-influential parameters to fixed values [Saltelli et al., 2009]. Moreover, an SA can enhance the understanding of the model parameters and can also assist in the identification of the model processes. In general, it can be stated that a sensitivity analysis can support the proper application of a complex environmental model.

A very powerful sensitivity analysis technique that is gaining popularity in environmental modelling is the variance-based Sobol’ method [Sobol’, 1990]. It is a global SA method that is model independent, i.e. it does not rely on preliminary assumptions about the model, such as linearity, additivity and monotonicity. Moreover, the Sobol’ SA also has other properties that are required for an ideal sensitivity analysis method, as it is able to cope with the influence of scale and shape, can account for interaction effects between parameters, yields quantitative results and can treat grouped parameters as if they were single parameters [Saltelli et al., 2009]. Additionally, the interpretation of the results is very intuitive and straightforward.

The high number of model evaluations necessary to perform the Sobol’ sensitivity analysis is however a major restriction for its use. Hence, an optimised convergence of the Sobol’ SA is of the utmost importance.

The sensitivity measures of the Sobol’ SA (i.e. the sensitivity indices) are assessed by means of Monte Carlo integrals. These numerical integrals are also used to compute an estimate of the square of the expectation value and the total variance of the model output. However, different formulas exist to estimate these statistics, which may have an impact on the computed sensitivity indices. The choice of the calculation method can highly affect the convergence of the sensitivity analysis results. Therefore, the main objective of this paper is to compare the influence of the various computation methods on the convergence of the SA results. To this end, we will use the Soil and Water Assessment Tool (SWAT) [Arnold et al., 1993] as an example of a complex, over-parameterized model.

2 MATERIALS AND METHODS

2.1 The SWAT model of the river Kleine Nete

A SWAT model of the Kleine Nete catchment (Belgium) with a daily time step has been employed as a case study for this research. The model of this relative small (580 km²) catchment has been used for the simulations of flow and nitrate concentration. 26 model parameters are considered. A full description of this model and the considered parameters is provided by Nossent et al. [2011]. More details on the semi-distributed, physically based Soil and Water Assessment Tool (SWAT) can be found in [Arnold et al., 1993; Gassman et al., 2007].

2.2 The Sobol’ sensitivity analysis

The core idea of the Sobol’ method [Sobol’, 1990] is to quantify the amount of variance that each of the $k$ parameters $X_i$ contributes to the unconditional variance of the output $V(Y)$. This contribution can either be caused by variations of an individual parameter (the main effect) or by interactions of a parameter with one or more other parameters. To account for the variance contribution of the parameters, the method is based on variance decomposition, which can be written as:
where \( V_i \) is the partial variance representing the main or first-order effect of \( X_i \) on the model output \( Y \). Similarly, \( V_{ij} \) is the partial variance corresponding with the second-order effect of interactions between parameters \( X_i \) and \( X_j \) on \( Y \) and \( V_{1,...,k} \) characterizes the interaction effect of all \( k \) parameters.

The variance contributions to the total output variance of individual parameters and parameter interactions are characterized by the ratio of the partial variances to the total unconditional variance, the Sobol’ sensitivity indices. The latter are the sensitivity measures of the Sobol’ SA.

First order SI
\[
S_i = \frac{V_i}{V} \tag{2}
\]

Second order SI
\[
S_{ij} = \frac{V_{ij}}{V} \tag{3}
\]

Total SI
\[
S_{Ti} = S_i + \sum_j S_{ij} + \cdots \tag{4}
\]

The calculation of \( S_{Ti} \) can be based on the variance \( V_{-i} \) that results from the variation of all parameters, except \( X_i \) [Homma and Saltelli, 1996]:
\[
S_{Ti} = 1 - \frac{V_{-i}}{V} \tag{5}
\]

For a complete background on variance based methods and the Sobol’ SA in particular, it is suggested to consult the work of Saltelli et al. [2009].

To compute the variances needed to obtain the sensitivity measures, Monte Carlo integrals are applied. The estimation of e.g. the total unconditional variance with this numerical integration technique then becomes:
\[
\hat{V}(Y) = \frac{1}{(N - 1)} \sum_{m=1}^{N} f^2(x^{(m)}) - \bar{f}^2 \tag{6}
\]

where \( \bar{.} \) stands for the estimate, \( f \) is the function representing the model (or objective function), \( x^{(m)} \) is a sampled set of the \( k \) parameters \( X_i \), \( N \) is the number of samples and \( \bar{f}^2 \) is the square of the expectation value of \( f \).

To compute the Monte Carlo integrals, Saltelli et al. [2010] suggest to use two independent \( N \times k \)-matrices (the “sample” matrix \( M_1 \) and the “resample” matrix \( M_2 \)). Every row in \( M_1 \) and \( M_2 \) represents a possible parameter combination for the model, symbolized as respectively \( x^{(1)(m)} \) and \( x^{(2)(m)} \).

Based on \( M_1 \) and \( M_2 \), different possibilities exist to estimate the square of the expectation value \( \bar{f}^2 \) and the total variance \( \hat{V} \). The most straightforward option to calculate \( \bar{f}^2 \) is to take samples of the “sample” matrix (equation (7)) or the “resample” matrix (equation (8)): 
\[
(f_0^{(1)})^2 = \left( \frac{1}{N} \sum_{m=1}^{N} f(x^{(1)}(m)) \right)^2
\]  
(7)

\[
(f_0^{(2)})^2 = \left( \frac{1}{N} \sum_{m=1}^{N} f(x^{(2)}(m)) \right)^2
\]  
(8)

Since the “sample” and “resample” matrices are independently sampled, the expectation value can also be estimated with samples from both \(M_1\) and \(M_2\):

\[
(f_0^{(1,2)})^2 = \left( \frac{1}{2N} \sum_{m=1}^{2N} f(x^{(1,2)}(m)) \right)^2
\]  
(9)

where \(x^{(1,2)}(m)\) is a set of parameters taken from the matrix \(M_{1,2}\), obtained by combining \(M_1\) and \(M_2\). Additionally, Homma and Saltelli [1996] suggested to use equation (10) as an estimate for the square of the expectation value for the computation of the first order index.

\[
(f_0^{(1x2)})^2 = \frac{1}{N} \sum_{m=1}^{N} f(x^{(1)}(m)) f(x^{(2)}(m))
\]  
(10)

In the same way, three different estimates for the total variance \(\tilde{\mathcal{V}}\) can be proposed based on \(M_1, M_2\) and \(M_{1,2}\) respectively:

\[
\tilde{\mathcal{V}} = \frac{1}{N-1} \sum_{m=1}^{N} f^2(x^{(1)}(m)) - f_0^2
\]  
(11)

\[
\tilde{\mathcal{V}} = \frac{1}{N-1} \sum_{m=1}^{N} f^2(x^{(2)}(m)) - f_0^2
\]  
(12)

\[
\tilde{\mathcal{V}} = \frac{1}{2(N-1)} \sum_{m=1}^{2N} f^2(x^{(1,2)}(m)) - f_0^2
\]  
(13)

In combination with the four options for the estimation of the square of the expectation value, this yields 12 possible formulas for the estimation of the total variance.

The Monte Carlo estimates of the partial variances \(\tilde{\mathcal{V}}_i\) and \(\tilde{\mathcal{V}}_{-i}\) become:

\[
\tilde{\mathcal{V}}_i = \frac{1}{N-1} \sum_{m=1}^{N} f(x^{(1)}(m)) f(x^{(2)}(m)) - f_0^2
\]  
(14)

\[
\tilde{\mathcal{V}}_{-i} = \frac{1}{N-1} \sum_{m=1}^{N} f(x^{(1)}(m)) f(x^{(2)}(m)) - f_0^2
\]  
(15)

where \(x^{(1)}(m)\) is a sample set from \(M_1\) of all parameters, except for \(X_i\) and \(x^{(1)}(m)\) is a sample from \(M_1\) of parameter \(X_i\). Similarly, \(x^{(2)}(m)\) is a sample set from \(M_2\) of all parameters, except for \(X_i\) and \(x^{(2)}(m)\) is a sample from \(M_2\) of parameter \(X_i\).
In total, the calculation of the first order and total Sobol’ sensitivity indices for all parameters requires $N \cdot (k + 2)$ model evaluations [Saltelli, 2002]. To sample $M_1$ and $M_2$, the Sobol’ quasi random sampling technique [Sobol’, 1967; 1976] is used.

### 2.3 The objective functions

Since the Sobol’ SA algorithm requires a single value for each model evaluation, the use of an objective function is essential to transform the time series of daily simulations (and observations) into a single value. For flow simulations, the Nash-Sutcliffe efficiency (NSE) [Nash and Sutcliffe, 1970] has been applied (see equation (16)).

$$\text{NSE} = 1 - \frac{\sum_t (y_{o,t} - y_{s,t})^2}{\sum_t (y_{o,t} - \bar{y}_o)^2}$$  \hspace{1cm} (16)

In this equation, $y_{o,t}$ is the observed value on day $t$, $\bar{y}_o$ is the average of the observations and $y_{s,t}$ is the simulated value on day $t$. The NSE value ranges from $-\infty$ (very bad model) to 1 (perfect model), with 0 indicating a model that can make predictions of the same quality as the mean of the observations.

However, the accuracy of the variance estimation (e.g. equation (6)) may decrease when the estimate of the square of the expectation value ($\bar{y}_o^2$) (e.g. equation (7)) becomes too large [Sobol’, 2001]. Although the values of $\bar{y}_o^2$ for flow simulations are relatively small for the NSE when compared to e.g. the also commonly used Sum of Squared Residuals (SSR), the application of the NSE for nitrate concentration simulations with our model yielded large values of $\bar{y}_o^2$, leading to inaccurate and even unrealistic results for the Sobol’ sensitivity indices. To overcome this problem, a normalized Nash-Sutcliffe efficiency (NNSE) (equation (17)) that yields values between 0 and 1 was introduced by Nossent and Bauwens [2012] and here applied for the Sobol’ SA of the nitrate concentration simulations.

$$\text{NNSE} = \frac{1}{1 + \frac{\sum_t (y_{o,t} - y_{s,t})^2}{\sum_t (y_{o,t} - \bar{y}_o)^2}} = \frac{1}{2 - \text{NSE}}$$ \hspace{1cm} (17)

For this objective function, the value 1 corresponds with the perfect model, 1/2 is the equivalent of an NSE value 0 and a very bad model is represented by a value of the normalized NSE of 0.

### 3 RESULTS AND DISCUSSION

According to Saltelli [2002], the sensitivity indices are best achieved by using equation (11) for the estimation of the total variance, in combination with equation (10) for $\bar{y}_o^2$ for the computation of the first order index and equation (7) for the total sensitivity index. To assess the influence of the 12 different combinations available for the estimation of the total variance and the square of the expectation value on the convergence of both the first order and total sensitivity indices, the evolution of the sum of the $S_T^2$ and $S_1^2$-values for all parameters with increasing sample size is investigated.
3.1 The convergence of the sensitivity indices for flow simulations

Figure 1 shows the sum of the first order sensitivity indices for flow simulations, as a function of the sample size and as calculated by different equations for the estimation of $\hat{V}$ and $f_o^2$. Four clusters of equations with a similar influence on the convergence of the first order sensitivity indices can be clearly identified. Within each of these clusters, the applied formula for the square of the expectation value is identical, pointing out that the estimate of $f_o^2$ is the main determining factor for the convergence of the first order sensitivity indices for flow simulations with the SWAT model.

![Figure 1](image1.png)

**Figure 1.** Evolution of the sum of the first order sensitivity indices for flow simulations with increasing sample size, for the 12 different combinations for the estimation of $f_o^2$ (denoted by (7), (8), (9), (10)) and $\hat{V}$ (denoted by (11), (12), (13)).

It can be noted from Figure 1 that the application of equation (9) yields much better results than the use of equations (7) and (8). The most stable evolution is however obtained by applying equation (10). This is in line with the suggestion of Saltelli [2002]. Nevertheless, he suggested to use equation (11) for $\hat{V}$, whereas in this case equation (13) yields a slightly better convergence.

Opposite to the results of the first order sensitivity indices, the estimate of $\hat{V}$ is the main determining factor for the convergence of $S_{Vf}$ for flow simulations (Figure 2).

![Figure 2](image2.png)

**Figure 2.** Evolution of the sum of the total sensitivity indices for flow simulations with increasing sample size, for the 12 different combinations for the estimation of $f_o^2$ (denoted by (7), (8), (9), (10)) and $\hat{V}$ (denoted by (11), (12), (13)).

Where Saltelli [2002] suggested to use equation (11), it is observed from Figure 2 that the set of combinations that employ equation (12) for estimating the total variance clearly yields the most stable evolution of the sum of $S_{Vf}$. In general, this is...
a similar configuration as proposed by Saltelli [2002], although the resample matrix (M_p) is used instead of the sample matrix (M_q). Furthermore, the combinations with equations (9) and (10) for $\hat{f}_n^2$ perform slightly better than sets with equations (7) and (8).

In general, it appears from the plots that a sample size of more than 12000 is required for the non-converged combinations to reach the final (converged) value.

### 3.2 The convergence of the sensitivity indices for nitrate concentration simulations

Similar observations as for the flow simulations can be made when nitrate concentrations are considered, instead of flow (Figure 3). Applying equation (10) for the estimation of $\hat{f}_n^2$ yields the most stable evolution of the sum of $S_{ij}$. Also the application of equation (9) seems beneficial for the convergence of the first order sensitivity indices. Again, the combination with equation (13) for $\hat{V}$ yields a slightly better convergence than the formulas (11) and (12).

![Figure 3. Evolution of the sum of the first order sensitivity indices for nitrate conc. simulations with increasing sample size, for the 12 different combinations for the estimation of $\hat{f}_n^2$ (denoted by (7), (8), (9), (10)) and $\hat{V}$ (denoted by (11), (12), (13))](image)

Although the general appearance of Figure 4 is different from Figure 2, the outcome of both graphs is very similar. The cluster of combinations that employ equation (12) for estimating $\hat{V}$ yields the most stable evolution of the sum of $S_{ij}$ for nitrate concentration simulations. In particular in combination with equations (9) and (10) for $\hat{f}_n^2$, the best convergence is observed for the total sensitivity indices.

![Figure 4. Evolution of the sum of the total sensitivity indices for nitrate conc. simulations with increasing sample size, for the 12 different combinations for the estimation of $\hat{f}_n^2$ (denoted by (7), (8), (9), (10)) and $\hat{V}$ (denoted by (11), (12), (13))](image)
4 CONCLUSIONS AND RECOMMENDATIONS

The comparison of the influence of various equations for the estimation of the total variance and the square of the expectation value on the evolution of the sum of the first order and total Sobol’ sensitivity indices with increasing sample size shows that the applied equations have a high influence on the convergence of the output of the Sobol’ method. Independently of the simulated variable and the applied objective function, the convergence of $S_i$ is mainly determined by the applied formula for $f_i^2$. Oppositely, the convergence of $S_{T_i}$ is highly affected by the applied equation for $P$.

For this case study the application of equations (10) and (13) for $S_i$ and equations (9) (or (10)) and (12) for $S_{T_i}$ yields the most stable evolution of the sensitivity indices with increasing sample size. It is, however, recommended to perform a similar assessment of the appropriate equations whenever the Sobol’ method is applied, as this takes less time than evaluating the model a number of times.

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