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Global sensitivity analysis for urban water quality modelling: Terminology, convergence and comparison of different methods

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ABSTRACT

Sensitivity analysis represents an important step in improving the understanding and use of environmental models. Indeed, by means of global sensitivity analysis (GSA), modellers may identify both important (*factor prioritisation*) and non-influential (*factor fixing*) model factors. No general rule has yet been defined for verifying the convergence of the GSA methods. In order to fill this gap this paper presents a convergence analysis of three widely used GSA methods (SRC, Extended FAST and Morris screening) for an urban drainage stormwater quality–quantity model. After the convergence was achieved the results of each method were compared. In particular, a discussion on peculiarities, applicability, and reliability of the three methods is presented. Moreover, a graphical Venn diagram based classification scheme and a precise terminology for better identifying important, interacting and non-influential factors for each method is proposed. In terms of convergence, it was shown that sensitivity indices related to factors of the quantity model achieve convergence faster. Results for the Morris screening method deviated considerably from the other methods. Factors related to the quality model require a much higher number of simulations than the number suggested in literature for achieving convergence with this method. In fact, the results have shown that the term "screening" is improperly used as the method may exclude important factors from further analysis. Moreover, for the presented application the convergence analysis shows more stable sensitivity coefficients for the Extended-FAST method compared to SRC and Morris screening. Substantial agreement in terms of factor fixing was found between the Morris screening and Extended FAST methods. In general, the water quality related factors exhibited more important interactions than factors related to water quantity. Furthermore, in contrast to water quantity model outputs, water quality model outputs were found to be characterised by high non-linearity.

1. Introduction

The evaluation of urban water quality represents a key issue in the urban drainage field in view of implementing environmental protection for receiving water bodies (Novotny et al., 1985). In this context mathematical models able to predict both water quantity and quality characteristics may provide useful support. Despite the fact that several water quality models are available in the urban drainage field, several aspects still limit their applicability, e.g. the extreme spatial and temporal variability of the water quality–quantity characteristics or the lack of distributed field data, which consequently forces modellers to impose a considerable number of assumptions. Due to these assumptions their predictions are characterised by high uncertainty (Beck, 1987; Ashley et al., 2005; Deletic et al., 2012; Dotto et al., 2012; Mannina and Viviani, 2010). One may ask whether and how these model assumptions influence the output of the model. In this context, sensitivity analysis represents a very powerful tool to provide answers, as it is able to determine how uncertain factors affect the model outputs (Saltelli et al., 2004). The term "factors" includes all the input variables and the model parameters that are varied during the sensitivity analysis.

Several sensitivity analysis methods have been proposed in literature, mainly divided into two groups: local sensitivity analysis methods and global sensitivity analysis methods (Saltelli, 2000). The local methods provide a measure of the local effect on the model output of a given model factor by evaluating the change

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in model outputs under small changes of the model factors. Global sensitivity analysis (GSA) methods assess how the model outputs are influenced by the variation of the model factors over their entire variation range (Homma and Saltelli, 1996; Saltelli et al., 2004). GSA may help modellers in selecting important factors (factor prioritisation), non-influential factors (factor fixing) as well as identifying interactions among factors and performing factors identifiability. More specifically, by means of "factor prioritisation" the model factors that have the largest effect on model outputs are identified. Conversely, the "factor fixing" setting leads to the identification of factors that may be fixed at any given value over their range without changing the output (Saltelli et al., 2004).

In Saltelli (2000) the GSA methods are classified into: (i) global screening methods, e.g. Morris screening method (Morris, 1991; Campolongo et al., 2007); (ii) variance decomposition methods such as Extended Fourier Amplitude Sensitivity Testing (Extended-FAST) (Saltelli et al., 1999); (iii) regression/correlation-based methods such as the standardised regression coefficients (SRCs) method (Saltelli et al., 2008). Due to the high complexity of environmental models, the spread of the GSA applications has been limited due to their high computational cost (Campolongo et al., 2007; Yang, 2011). Therefore, modellers have often been reluctant to use GSA methods instead of local methods (Saltelli and Annoni, 2010). Despite such problems in applying GSA, during the last years modellers have spent considerable time in understanding the potentialities of each GSA method applied to complex models, especially in some areas such as hydrology (e.g., Massmann and Holzmann, 2012; Herman et al., 2013; Zhan et al., 2013).

1.1. Comparison of GSA methods

In Table 1 all the relevant studies on GSA found in literature are summarised. They are discussed below.

Some authors have compared the different GSA methods in order to highlight the potential of each method and the differences of the results.

Tang et al. (2007) compared four sensitivity analysis methods for a watershed model with 18 factors. In particular they applied one local sensitivity analysis method (Parameter Estimation Software, PEST) and three global sensitivity analysis methods (Regional Sensitivity Analysis – RSA; Analysis of Variance – ANOVA and Sobol's method). Convergence for the RSA and Sobol' methods was tested on the basis of the values of the sensitivity indices and on the reproducibility of the results. For the PEST method the authors imposed a maximum value of 30 iterations for each model factor. They found that, in terms of sensitivity classification, the results of the PEST method were significantly different compared to the other three methods due to the local nature of the PEST application. Moreover, among the three global methods, the Sobol' method was considered the most robust in terms of sensitivity rankings, detailed in terms of variance decomposition and easy to interpret.

Yang (2011) compared five different sensitivity analysis methods (Sobol', Morris screening, Linear Regression, RSA and SDP non-parametric regression/smoothing approach) for a hydrological model of the Leaf River watershed with five model factors. On the basis of the Central Limit Theorem the author established the achievement of convergence for the sample size for which no significant change in the coefficient of variance occurred. The author found similar results in terms of parameter ranking for the Sobol', Morris screening and Linear Regression methods and for the SDP non-parametric regression/smoothing approach. The different results obtained with the RSA were attributed to the choice of the filtering criteria.

Sun et al. (2012) compared three sensitivity analysis methods of a hydrological water quality model with 6 model factors: the local method, the Morris screening method and RSA. They concluded that the compared methods should be considered as complementary and not as mutually exclusive alternatives. The peculiar features of each method can assist the modeller in characterising the behaviour of the model studied. In case of a model with a large number of factors, Sun et al. (2012) suggested to use a two-step procedure including first a factors screening step (by using a local method) followed by a global sensitivity analysis step of the important factors identified during the first step.

Neumann (2012) presented a comparison among five sensitivity analysis methods (derivative-based local sensitivity analysis, Morris screening, Standardised Regression Coefficients, Extended-FAST and an entropy-based method) for a model predicting micropollutant degradation in drinking water treatment with 10 model factors. Although the author found the same parameter ranking for the different methods he underlined the poor approximation of 1st order effect indices obtained with the local methods or regression-based methods. Thus, when model non-linearity increases the factors classification can significantly differ when local methods or regression-based methods are applied.

Recently, Cosenza et al. (2013) compared three global sensitivity analysis methods (SRC, Morris screening and Extended FAST) to assess the most relevant processes occurring in membrane bioreactor wastewater treatment systems by using the numerical settings as suggested in literature. Morris screening and Extended-FAST showed low similarity in terms of both the number and type of influential/non-influential factors. The differences were attributed to convergence problems for the Morris screening results. Further, very similar results were obtained between the Extended-FAST and SRC methods despite the fact that SRC was applied outside its range of applicability ($R^2 < 0.7$). Thus, Cosenza et al. (2013) suggested, for the case studied, to use the SRC method (less computationally demanding compared to the Extended FAST method) in case the modeller is only interested in *factor prioritisation*.

1.2. Convergence analysis

Despite the aforementioned reports on the convergence issues for the GSA results, only few studies regarding the assessment of convergence exist in literature (e.g., Benedetti et al., 2011; Yang, 2011; Wang et al., 2013). Benedetti et al. (2011) proposed a method to minimise the computational cost of Monte Carlo based GSA methods in the wastewater treatment modelling field. They focused their attention on two criteria (the model output variability and the stability of the composition of the important factor set as the number of iterations increases) for selecting the minimum number of simulations to be performed. However, they found that by using different criteria the results of the convergence analysis are quite different highlighting that the achievement of convergence is strongly dependent on the model output considered during GSA application. Benedetti et al. (2011) suggested that the number of simulations required to reach convergence is between 40 and 150 times the number of uncertain model factors. Such a result is not in line with the findings of previous works where the maximum value of 50 times (the number of uncertain model factors) was suggested (Benedetti et al., 2010).

Yang (2011) proposed a method to investigate the convergence of the results of different Monte Carlo based GSA methods by using two techniques for monitoring the convergence: the Central Limit Theorem (CLT) and the bootstrap technique. Yang (2011) found, for a simple model characterised by 5 factors, that for each GSA method the bootstrap technique leads to a lower number of simulations required than the CLT. Further, Nossent and Bauwens