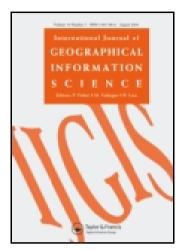
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Research Article

Sensitivity analysis of spatial models

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Sensitivity analysis is the study of how uncertainty in model predictions is determined by uncertainty in model inputs. A global sensitivity analysis considers the potential effects from the simultaneous variation of model inputs over their finite range of uncertainty. A number of techniques are available to carry out global sensitivity analysis from a set of Monte Carlo simulations; some techniques are more efficient than others, depending on the strategy used to sample the uncertainty of model inputs and on the formulae employed for estimating sensitivity measures. The most common approaches are summarised in this paper by focusing on the limitations of each in the context of a sensitivity analysis of a spatial model. A novel approach for undertaking a spatial sensitivity analysis (based on the method of Sobol' and its related improvements) is proposed and tested. This method makes no assumptions about the model and enables the analysis of spatially distributed, uncertain inputs. The proposed approach is illustrated with a simple test model and a groundwater contaminant model.

Keywords: Uncertainty analysis; Sensitivity analysis; Spatial models, Nitrate transport

1. Introduction

Models of varying complexity are developed to describe, at a given degree of approximation, systems and processes in different aspects of the real world (e.g. industrial, environmental, social, or economic). The use of models, in particular in the environmental domain, inevitably involves the presence and treatment of uncertainties. The input to a model is subject to many sources of uncertainty including errors of measurement, the absence of information, sampling design, out-of-date information, scaling errors, and poor or partial understanding of the driving forces and mechanisms (model conceptual uncertainty) (Burrough and McDonnell 1998). This imposes a limit on our confidence in the response of the model. Uncertainty and sensitivity analyses are potentially able to increase confidence in the model and its predictions, by providing an understanding of how the model response variable(s) respond to changes in the inputs.

While uncertainty analysis quantifies the magnitude of the resulting uncertainty in the model predictions due to uncertainties in model inputs, sensitivity analysis (SA) is the study of how the uncertainty in the output of the model can be apportioned to different sources of uncertainty in the model inputs (Saltelli *et al.* 2004). Uncertainty and sensitivity analysis can serve a number of useful purposes in the process of model building and use. These include corroborating the model structure, identifying critical regions in the space of the inputs, determining minimum data standards, and establishing priorities for updating the model (including model simplification).

A number of SA techniques have been developed, many of which involve repeatedly running the model in a Monte Carlo approach (Saltelli *et al.* 2000). However, this procedure becomes computationally more difficult, or even intractable, when temporally and/or spatially distributed inputs are considered. In addition to the computational problems, there are also some conceptual issues in applying many of the SA techniques to a spatial model. These include the difficulties in satisfying key assumptions inherent in some of the techniques, the need to represent a spatial input with a scalar value, and the desirability of being able to simulate auto-correlated inputs and analyse the effect of spatial structure. Alternatively, an analytical approach to SA, e.g. based on a Taylor series approximation, can be difficult to implement, and is confined to a local analysis of the input/output relationship. Consequently, SA of spatial models is often either ignored or is relatively limited in scope.

This paper summarises the various approaches that have been used to get around the computational and conceptual problems of performing a Monte Carlo-type SA on spatial models. The limitations of these various approaches are discussed, and the method of Sobol' (and its generalisations), adapted to the case of spatial models, is presented and tested on two case studies.

2. Background: sensitivity analysis techniques

Different SA techniques are characterised by different properties, computational cost, and application scope. A thorough review of techniques for SA is given by Saltelli *et al.* (2000) and in Helton (1993). The main approaches are briefly summarised here.

The aim of local sensitivity analysis is to quantify the rate of change of the model output due to small variations in the uncertain model inputs. This quantification relies on derivatives that are calculated at specific points in the space of the inputs. However, the choice of the point can largely influence the outcomes of the sensitivity analysis, especially when the space of the input is affected by considerable uncertainty. This constitutes a very limited assessment for non-linear models. A review of deterministic sensitivity analysis methods is given by Turanyi and Rabitz (2000).

Global sensitivity analysis methods consider the full ranges of uncertainty of the inputs, which are characterised via their joint probability density functions (pdf). Often, the inputs are considered independent, and their marginal pdfs are sufficient to characterise their uncertainty. In a global SA, all the inputs are varied simultaneously, and multi-dimensional averaging is used to quantify interactions among them. A global SA follows six steps:

- (1) Specify the target function of the study
- (2) Select the inputs of interest
- (3) Assign a range and a statistical distribution to the selected inputs
- (4) Apply a sampling design to generate a sample of size N from the distributions of the inputs
- (5) Evaluate the model for each sample set of input values obtaining N values for the target function

(6) Use the results of step 5 for uncertainty analysis and apply an estimator of sensitivity to obtain the relative importance of the inputs

The ranges and distributions in step 3 are deduced from available information, such as available data, physical bounding considerations, expert opinion, or through parameter estimation in inverse problems. If the analysis is exploratory, then rather crude assumptions may be adequate. The sample generation (step 4) can be accomplished in a number of ways, as several sampling designs are available. The simplest way is to use Monte Carlo random generation algorithms from the assigned distributions (e.g. simple random sampling, SRS). Other more refined sampling techniques include Latin hypercube sampling (LHS), quasi-random sequences (Sobol' 1967), winding stairs (Jansen *et al.* 1994), replicated LHS (McKay 1995), Fourier Amplitude Sensitivity Test (FAST) (Cukier *et al.* 1978), extended FAST (Saltelli *et al.* 1999), and random balance designs (Tarantola *et al.* 2006a). Such sampling strategies need their correspondent estimator to be able to obtain sensitivity measures for the inputs (see Figure 1 for the various combinations). Some of the sampling techniques rely on a reordering scheme which effectively resamples from a set of realisations (e.g. random balance designs and replicated LHS).

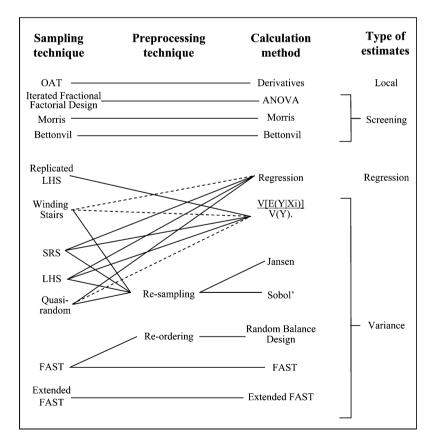


Figure 1. Diagram showing which sampling techniques and sensitivity estimation methods can be combined. Dashed lines show combinations that have not been used in literature to date. See Saltelli *et al.* (2000) for further information on the techniques.

Methods are also available for generating dependent samples when the problem requires it (see, e.g. Stein 1987). However, in such cases, estimation of the sensitivity measures can become burdensome.

In step 6 above, screening, regression, and variance-based measures can be obtained.

For computationally expensive models with often a large number of inputs, screening experiments are computationally affordable techniques that are used to identify the inputs that have little effect on the output variability. These inputs can therefore be fixed in subsequent analyses (to their mean value, for instance) without significantly modifying the prediction characteristics of the model. The most common screening technique is that proposed by Morris (1991), which has recently been improved by Campolongo *et al.* (2007).

In a regression-based approach, a linear regression model linking the inputs to the output is fitted to the available points obtained from the Monte Carlo simulations. The coefficients of the regression model are estimated through ordinary least squares (Saltelli *et al.* 2000).

Variance-based methods have the capability to compute sensitivity indices regardless of the linearity or monotonicity, or other generic assumptions on the underlying model. In variance-based methods, the variance V of the model prediction is decomposed into partial variances which represent the share of V that is explained by the model inputs (either considered singularly or in combination) and therefore the importance of the inputs themselves

$$V = \sum_{i} V_{i} + \sum_{i < j} V_{ij} + \sum_{i < j < m} V_{ijm} + \dots + V_{12\dots k}$$
 (1)

where V_i is the share of the output variance explained by the *i*th model input, and represents the sensitivity of Y to X_i ; V_{ij} is the share of the output variance explained by the interaction of the *i*th and *j*th inputs, and represents the sensitivity of Y to the interaction between X_i and X_i ; k is the total number of model inputs.

The first-order sensitivity indices $S_i = V_i/V$ can be written in terms of conditional variances:

$$S_i = \frac{\operatorname{Var}[E(Y|X_i)]}{\operatorname{Var}(Y)} \tag{2}$$

The inner expectation of the numerator is conditional on X_i taking a value X_i^* within its range of uncertainty. The outer variance is calculated over all possible values of X_i ; this calculation requires the knowledge of the inner expectation at all X_i^* , which requires, for each X_i^* , the calculation of an integral in k-1 dimensions; this would be extremely expensive if specific techniques, like Sobol's, were not available. The denominator is the unconditional variance of the model output Y and its computation is straightforward. Variance-based methods have been applied in many areas, including neural computations (Castillo *et al.* 2007), food safety assessment (Patil and Frey 2004), and solid state physics (Pastorelli *et al.* 2000).

3. Approaches for spatial sensitivity analysis (SSA)

3.1 Review of approaches

A number of approaches can help simplify the dimensionality or reduce the computational demands of an SSA. These are now explained and discussed in terms of the constraints and disadvantages of each.

If the model under investigation has a spatially distributed output, then an appropriate scalar objective function is selected to base the SA upon (such as an aggregated statistic like sum, average, maximum value, expected cost, maximum risk, or annual river flow at the outlet of a catchment). Alternatively, if no aggregated scalar can be identified as the objective function, then the SA should be repeated for every unique polygon or pixel independently (e.g. Lodwick *et al.* 1990; Bekesi and McConchie 1999). This could result in a cumbersome number of sensitivity indices for each model input, and the effect of spatial autocorrelation and structure cannot be analysed.

A one-at-a-time approach (OAT) is the most common method in which one input parameter at a time is selectively varied to determine its effect on the objective function (e.g. Walsh $et\ al.$ 1994). Each input might be varied by a given amount, e.g. ± 10 or 20% (Swartzman and Kuluzny 1987), spatially swapping a varying proportion of the cells (Fisher $et\ al.$ 1997), or shifting locations according to a probability distribution (Stoms $et\ al.$ 1992). This method is local and OAT (Lodwick $et\ al.$ 1990) in that the other parameters are not varied but fixed at nominal values, and the SA is limited to a small area of the parameter space. It follows that the SA tends to be relatively informal and $ad\ hoc$ and the results are not generally valid.

A global SSA was proposed by Crosetto *et al.* (2000) and Crosetto and Tarantola (2001) where the extended FAST technique (Saltelli *et al.* 1999) was applied. However, Crosetto and Tarantola (2001) implemented very rudimentary and non-realistic spatial uncertainty models. For example, the various realisations of the uncertainty model for a rainfall map were obtained as spatially uniform maps. The nominal rainfall map values were varied by $\pm z$, where z was a scalar uncertainty source sampled from a uniform distribution.

The model parameters used in Tang *et al.* (2007b) were also spatially lumped (i.e. every grid cell takes the same value for a specific parameter) in order to make the Sobol' method computationally tractable. In another case study, Tang *et al.* (2007a) considered spatially distributed parameters; however, the Sobol' measures were calculated for each model cell independently.

Another approach to spatial uncertainty modelling by Hall *et al.* (2005) simplified the spatial dimension by reducing the spatial variability to just a few zones, each of which was characterised by a set of scalar inputs. They used this approach to determine the most critical river reach in a flood inundation problem. The region was divided into four sub-regions, each with its own set of scalar inputs, which were combined in a global SA. No spatial uncertainty model was employed within each sub-region. This approach is suitable if the number of spatial regions with different values is very small (e.g. four in the case of Hall *et al.* 2005).

A variation of this spatial simplification approach is to randomly, or purposefully, select a small representative set of pixels or points, and carry out an SA on each point (e.g. Avissar 1995; Dubus and Brown 2002; Lilburne *et al.* 2003). A cluster analysis might be used to identify pixels that are the most dissimilar in attribute space, suggesting different SA results. The effects of spatial autocorrelation and spatial structure on model output cannot be analysed in this approach.

If spatial variation is sufficiently regular and well behaved that it can be successfully modelled as a statistical model with a small number of parameters, then these parameters can be considered as input factors in the SA. For example, spatial variability might be described by statistical moments, e.g. mean, standard deviation, skewness, or other shape parameters. This approach has been proposed and used by Kioutsioukis *et al.* (2004) in dealing with both temporal and spatial data.

Lilburne *et al.* (2003) associated values sampled from a discrete, uniformly distributed input, with sample realisations from a pre-generated sequence of 1000 realisations of a set of soil maps. This enabled a complex correlated description of variability in soil profile data to be simulated that was not possible with other more common approaches. However, it was essential to sort the sequence according to the objective function so that the input had some 'meaning' when analysed with the regression or other SA techniques. This requirement to sort the sequence of spatial realisations so that the associated scalar input values have some meaning with respect to the objective function limits the utility of the approaches based on regression and the Fourier-based techniques (FAST).

In particular, both in regression and FAST, if the order in which spatial realisations are associated with the scalar input values is modified, the estimates of the coefficients of the regression model would be affected because these techniques aim at building an analytical relationship between input and output. Note also that FAST does not work properly when inputs are not continuous in their ranges. This fact would cause a break in the Fourier-based trajectories in the input space (for a discrete set of input values, there would be many pieces of trajectories and the Fourier coefficients will not be estimated properly).

Crosetto and Tarantola (2001) proposed the use of a binary input to 'switch' uncertainties on and off at the same rate (i.e. for N/2 runs, the switch is set to off and for the remaining N/2 runs it is set to on), allowing their relative importance to be determined. Geostatistical or other techniques can then be used to generate realisations from spatial uncertainty models that are then applied in 50% of the model runs. In the other 50%, the error layer is ignored. The SA is performed on the binary input. The simple example described below shows that while a result indicating that the 'switched' uncertainty is not an important input is probably reliable, this is not the case for an input that is found to be important (Table 1). This is because when the switch is set to on, the model undergoing the SA includes an additional stochastic source of uncertainty that modifies the model itself.

A simple method of achieving a global SA of non-spatial models is described by Vose (1996). Each input is fixed in turn while the others are varied. Total variance of the objective function is obtained by varying all inputs. The measure of input X_i 's importance is the relative drop in variance of the objective function due to this input being fixed (the bigger the drop, the more sensitive it is). This method could be extended to the spatial context, which would allow the simulation of a spatial uncertainty model. However, this approach is computationally very inefficient, because it requires each input to be fixed to a number of different values (or maps) within its range. Also, it is possible that having fixed an input, the conditional output variance could be higher than the total unconditional variance (Saltelli *et al.* 2004).

Table 1. Sensitivity indices for each parameter in a model $Y = X_1 + X_2 + X_3$ where X_3 is represented by a binary switch. The uncertainty of X_1 , X_2 and X_3 is U[0, 1]. All three variables are equally sensitive in the model (i.e. 0.33), but using a switch for X_3 lessens the first-order sensitivity of X_3 and increases the total-order sensitivity of X_1 and X_2 .

Parameter	First-order	Total-order	
$\overline{X_1}$	0.3	0.46	
X_2	0.3	0.45	
X_3 (switch)	0.21	0.38	

All of the approaches listed above have significant limitations (which are summarised in Table 2). Ideally, a spatial SA should combine a global approach, in which all inputs of interest are varied simultaneously and efficiently, with the ability to generate auto-correlated realisations of the input maps through appropriate geostatistical techniques. The SA approach should then work on the realisations of the input maps rather than on individual pixels or polygons, or representative scalar values, thus allowing the entire spatial structure to be accounted for in the analysis of the importance of each spatial input.

In this paper, the method of Tarantola *et al.* (2006b), a generalisation of the methods of Sobol' (1993) and Saltelli (2002), is applied to spatially dependent models, which has not to our knowledge been carried out before. Unlike the approaches discussed earlier, this approach does not constrain or limit the preparation of the input sample. For the *i*th input, scalar values sampled from X_i are associated with realisations generated from a spatial uncertainty model. This means that a complex auto-correlated spatial uncertainty model can be used to generate the spatial realisations, and the effect of spatial structure can be analysed. In addition, an analytical model to link input and output is not required as the described methods provide an estimate of the variance of the expectation of the model output Y conditional on the model input X_i , i.e. $V[E(Y|X_i)]$. This estimate does not depend on the order in which the realisations are associated with the scalar input values.

Another global approach with these advantages is the winding stairs/Jansen technique (Jansen *et al.* 1994). It has been applied to a spatial model on soil acidification by Kros *et al.* (1999).

3.2 The method of Sobol' and the derivations by Saltelli (2002) and Tarantola et al. (2006b)

The method of Sobol' provides appropriate formulae to estimate the terms in the decomposition of the output variance given in equation (1). The computational strategy of the method of Sobol' is the following:

- Choose an integer N (operational details are discussed in Section 5).
- Generate a matrix (N, 2k) of quasi-random numbers. Split the matrix in two
 matrices A and B of size (N, k). The columns of A and B are samples of the
 model inputs, extracted from their respective probability distributions.
- Define a matrix D_i formed by all columns of A, except the ith column, which is taken from B, and a matrix C_i formed with the ith column of A and with all the remaining columns of B (Figure 2).
- Compute the model output for all the input values in the matrices A, B, C_i and D_i , obtaining four vectors of model outputs of dimension $N \times 1$

$$\mathbf{y}_{A} = f(A), \, \mathbf{y}_{B} = f(B), \, \mathbf{y}_{C_{i}} = f(C_{i}), \, \mathbf{y}_{D_{i}} = f(D_{i})$$
 (3)

The method of Sobol' estimates first-order sensitivity indices as follows

$$\hat{S}_{i} = \frac{\hat{V}_{i}}{\hat{V}} = \frac{\hat{V}_{X_{i}} \left[\hat{E}_{\mathbf{X}_{-i}}(Y|X_{i}) \right]}{\hat{V}} = \frac{\mathbf{y}_{A} \cdot \mathbf{y}_{C_{i}} - \hat{f}_{0}^{2}}{\mathbf{y}_{A} \cdot \mathbf{y}_{A} - \hat{f}_{0}^{2}} = \frac{\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)} y_{C_{i}}^{(j)} - \hat{f}_{0}^{2}}{\frac{1}{N} \sum_{i=1}^{N} \left(y_{A}^{(j)} \right)^{2} - \hat{f}_{0}^{2}}$$
(4)

Table 2. Advantages and disadvantages of the various sensitivity analysis (SA) techniques in the context of a spatial SA.

Technique	Advantages	Disadvantages	Computationa demand
OAT	Simple	Local SA only	Very low
	•	Results reliable only if the model is linear	•
Morris	Can work with large models	Results are less accurate than the SA methods below	Low
	Computationally cheap	Sample generation is not straightforward	
Regression	Simple and straightforward	Results depend on goodness of fit of linear response model	Moderate
		Input parameters should be independent	
		Does not handle spatially variable inputs	
Random	Model independent	First-order effects only	Moderate
palance design		Not applicable when parameters have discontinuities	
		Input parameters should be independent	
~		Does not handle spatially variable inputs	
Classic and	Model independent	Not applicable when parameters have discontinuities	High
xtended FAST	Total-effect indices (only for extended FAST)	Input parameters should be independent	
*** **		Does not handle spatially variable inputs	*** 1
Winding	Model independent	Input parameters should be independent	High
stairs/Jansen	Total-effect indices	Specific sampling strategy required (usually winding stairs)	
	High-order interactions		
	Can have spatial input that is auto-correlated		
Sobol'	Spatial structure included in SA	Toward and an advantage of confidence of the first form of the design of the first form of the first f	TT! .1.
30001	Model independent Total-effect indices	Input parameters should be independent	High
	High-order interactions	Specific sampling strategy (usually quasi-random points)	
	Extension (using symmetries) makes this more		
	efficient		
	Can have spatial input that is auto-correlated		
	Spatial structure included in SA		
mportance	Model independent	Specific sampling strategy (usually replicated Latin Hypercube)	Very high
neasure	Works with dependent inputs	First-order effects only	, cry mgn
11043410	Can have spatial input that is auto-correlated	Computationally demanding	
	Spatial structure included in SA	companient demanding	

where the 'dot' indicates the scalar product between two vectors, E_{X-i} is the conditional expectation obtained by considering fixed values for X_i , and

$$\hat{f}_0^2 = \left(\frac{1}{N} \sum_{j=1}^N y_A^{(j)}\right)^2 \tag{5}$$

indicates the estimated average.

• Similarly, the method estimates total-effect indices as follows

$$\hat{S}_{Ti} = 1 - \frac{\hat{V}_{-i}}{\hat{V}} = 1 - \frac{\hat{V}_{\mathbf{X}_{-i}} \left[\hat{E}_{\mathbf{X}_{i}} (Y | \mathbf{X}_{-i}) \right]}{\hat{V}} = 1 - \frac{\mathbf{y}_{A} \cdot \mathbf{y}_{D_{i}} - \hat{f}_{0}^{2}}{\mathbf{y}_{A} \cdot \mathbf{y}_{A} - \hat{f}_{0}^{2}} = 1 - \frac{\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)} y_{D_{i}}^{(j)} - \hat{f}_{0}^{2}}{\frac{1}{N} \sum_{j=1}^{N} \left(y_{A}^{(j)} \right)^{2} - \hat{f}_{0}^{2}}$$
(6)

In summary, with a set of (2k+2)N simulations (where k is the number of model inputs and N the size of the base sample), one estimate of first-order index and one estimate of total effect can be obtained for each input.

Saltelli (2002) suggested that, rather than using equation (5), f_0^2 can be better estimated as

$$f_0^2 = \left(\frac{1}{N} \sum_{j=1}^N y_A^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^N y_B^{(j)}\right) \tag{7}$$

i.e. as products of independent vectors y_A and y_B . Therefore, an estimate of first-order effect is given by

$$S_{i}^{Saltelli\ I} = \frac{\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)} y_{C_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)}\right)}{\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)} y_{A}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)}\right)}$$
(8)

Saltelli (2002) exploited the symmetry between $\mathbf{y}_A \mathbf{y}_{C_i}$ and $\mathbf{y}_B \mathbf{y}_{D_i}$, and proposed another estimate for the first-order effect

$$S_{i}^{Saltelli\ II} = \frac{\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)} y_{D_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)}\right)}{\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)} y_{B}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)}\right)}$$
(9)

$$A = \begin{bmatrix} x_{1}^{(1)} & \cdots & x_{i}^{(1)} \\ x_{1}^{(2)} & \cdots & x_{i}^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1}^{(N)} & \cdots & x_{i}^{(N+1)} & \cdots & x_{k}^{(N+1)} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1}^{(N)} & \cdots & x_{i}^{(N+1)} & \cdots & x_{k}^{(N+2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1}^{(2N)} & \cdots & x_{i}^{(2N)} & \cdots & x_{k}^{(N+2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1}^{(N+1)} & \cdots & x_{i}^{(N+2)} & \cdots & x_{k}^{(N+2)} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{1}^{(N)} & \cdots & x_{i}^{(N)} & \cdots & x_{k}^{(N+1)} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{1}^{(N)} & \cdots & x_{i}^{(N)} & \cdots & x_{k}^{(N+2)} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{1}^{(2N)} & \cdots & x_{i}^{(N)} & \cdots & x_{k}^{(N)} \end{bmatrix}$$

Figure 2. Generating matrices C_i and D_i from A and B.

Tarantola et al. (2006b) proposed an alternative to estimate f_0^2

$$f_{0_i}^2 = \left(\frac{1}{N} \sum_{j=1}^N y_{C_i}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^N y_{D_i}^{(j)}\right)$$
(10)

i.e. using products of y_{Ci} and y_{Di} , which are also independent vectors (note that in this case, the estimate of f_0^2 depends on i). In this way, the denominator of equation (4) can be obtained either from $\frac{1}{N} \sum_{i=1}^{N} \left(y_{C_i}^{(j)} \right)^2 - \hat{f}_{0_i}^2$ or $\frac{1}{N} \sum_{i=1}^{N} \left(y_{D_i}^{(j)} \right)^2 - \hat{f}_{0_i}^2$.

Consequently, Tarantola *et al.* (2006b) proposed six additional estimates of first-order indices without the need of extra model simulations. The operational formulas for these additional estimates are reported next for transparency and to facilitate implementation of the technique

$$S_{i}^{Tarantola\ I} = \frac{\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)} y_{C_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)}\right)}{\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)} y_{B}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)}\right)}$$
(11)

$$S_{i}^{Tarantola~II} = \frac{\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)} y_{C_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{C_{i}}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{D_{i}}^{(j)}\right)}{\frac{1}{N} \sum_{j=1}^{N} y_{C_{i}}^{(j)} y_{C_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{C_{i}}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{D_{i}}^{(j)}\right)}$$
(12)

$$S_{i}^{Tarantola~III} = \frac{\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)} y_{C_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{C_{i}}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{D_{i}}^{(j)}\right)}{\frac{1}{N} \sum_{j=1}^{N} y_{D_{i}}^{(j)} y_{D_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{C_{i}}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{D_{i}}^{(j)}\right)}$$
(13)

$$S_{i}^{Tarantola~IV} = \frac{\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)} y_{D_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)}\right)}{\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)} y_{A}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{A}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)}\right)}$$
(14)

$$S_{i}^{Tarantola\ V} = \frac{\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)} y_{D_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{C_{i}}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{D_{i}}^{(j)}\right)}{\frac{1}{N} \sum_{j=1}^{N} y_{C_{i}}^{(j)} y_{C_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{C_{i}}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{D_{i}}^{(j)}\right)}$$
(15)

$$S_{i}^{Tarantola\ VI} = \frac{\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)} y_{D_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{C_{i}}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{D_{i}}^{(j)}\right)}{\frac{1}{N} \sum_{j=1}^{N} y_{D_{i}}^{(j)} y_{D_{i}}^{(j)} - \left(\frac{1}{N} \sum_{j=1}^{N} y_{C_{i}}^{(j)}\right) \left(\frac{1}{N} \sum_{j=1}^{N} y_{D_{i}}^{(j)}\right)}$$
(16)

The average of the eight sensitivity estimates in equations (8), (9), (11)–(16), which are positively and negatively correlated in pairs, is generally more accurate than the single estimates produced by equation (4) (the original Sobol's), or equations (8) or (9), at a given N.

Tarantola *et al.* (2006b) also exploited symmetry properties for equation (6), obtaining four estimates of total-effect sensitivity indices at no additional cost. The average across the four correlated estimates generally provides more accurate results than the single estimate from equation (6), at a given N.

In this work, we will use the average value among the eight first-order indices for X_i , which we denote simply by S_i , and the mean value among the four total-effect indices for X_i , which we denote by S_{T_i} .

These sensitivity indices can be estimated in a spatial context by simply associating realisations of spatially distributed uncertainty maps with random values sampled from scalar model inputs X_i . The realisations of spatial uncertainty maps, either with or without autocorrelation, can be generated by any method including geostatistical simulation routines. The sampling from the scalar model inputs X_i is performed either via standard random sampling or by using the more efficient quasi-random sampling strategy.

4. Application of the Sobol' method (and extensions) in an SSA

4.1 Test example 1

A simple weighted composite index model is used to demonstrate this approach. This is a model in the form of

$$Index = \sum_{i=1}^{n} w_i X_i \tag{17}$$

where w is the weight for each input variable i and n is the number of input variables.

For example, DRASTIC (Aller et al. 1987) is a weighted composite index that has been applied in a spatial context to rate the intrinsic vulnerability of land to groundwater contamination. Empirical models based on linear regression also take this form. In this demonstration, the objective function is defined as the mean $\overline{M}_{\text{out}}$ of the values in the output map M_{out} where M_2 and M_4 are spatially distributed uncertain maps, X_5 is an uncertain scalar input and w_1 and w_3 are uncertain weights

$$M_{out} = w_1 M_2 + w_3 M_4 + X_5 \tag{18}$$

The maps M_2 and M_4 , and the corresponding output map $M_{\rm out}$, are small raster maps or grids of 10×10 resolution. For each of M_2 and M_4 , a set of 100 realisations is generated and stored for the subsequent sensitivity analysis. This number of realisations is considered sufficient in this case to characterise the overall uncertainty of the spatially distributed maps. The particular map realisation to be used in a given model run will be selected by sampling at random an integer value between 1 and 100 (which is the model input for the respective spatial map).

Note that in practical cases, it might be difficult and expensive to generate and store so many realisations for each map input, and the analyst might have to consider a reduced number of realisations. If the analyst wants to determine the effect of maps derived from different sources or based on different classification algorithms for example, then only a few realisations may be needed.

The five model inputs of the test case are independent and their uncertainty properties are defined in Table 3. For example, the map M_2 in the base case is characterised by the distribution U[0, 5]. This could represent the case of a homogeneous average rainfall field of $2.5 \,\mathrm{cm}\,\mathrm{d}^{-1}$ over the spatial region, subject to an uncorrelated and uniformly distributed spatial uncertainty in the range [-2.5, 2.5] cm d⁻¹ over each pixel.

The first-order and total-effect sensitivity measures for the five inputs are estimated in a simulation that employed a simple random sampling strategy where N=10,000, which corresponds to a computational cost of N(2k+2)=120,000 model runs. We can afford such a high number of model runs, as the time to run this simple model is negligible. The results, reported in Table 3, show that the most important input (given the defined variability) is X_5 , with a first-order sensitivity of 60%, and the two weights are next in importance at 15% each. The two maps are the least critical, with approximately 5% individual contribution to the output variance, although the uncertainty associated with the maps is not insignificant. The sum of the first-order indices is 100% indicating that there is no interaction between the inputs (this is also confirmed by the fact that the estimates of the first- and total-order indices are practically the same), even though pairs of inputs are coupled in the model (i.e. a weight is multiplied by a map).

The uncertainties of some of the inputs are then varied to see whether the results change as expected (Tables 4–5). Increasing the uncertainty of w_1 increases the sensitivity of this input to 41.4%. Maintaining the range of variability but shifting the values of w_1 downwards with respect to the base case results in a reduced sensitivity for M_2 and no change in the sensitivity of w_1 . This is as expected, as with a lower weight the uncertainty of M_2 has less impact on \bar{M}_{out} .

Increasing the amplitude of the uncertainty affecting M_2 from U[0, 5] to U[0, 10] results in increasing the sensitivity of both M_2 and w_1 . With a higher average value of M_2 , the associated weight, w_1 , has more influence. Shifting the amplitude of the

Variable	Pdf	Sobol' estimate of first-order sensitivity (%) 10×10	Sobol' estimate of total-order sensitivity (%) 10×10	Sobol' estimate of first-order sensitivity (%) 50 × 50	Sobol' estimate of total-order sensitivity (%) 50 × 50
$\overline{w_1}$	U[0.5, 0.7]	15.4	15.5	16.3	16.3
M_2	U[0, 5]	4.7	4.8	0.2	0.2
w_3	U[0.5, 0.7]	15.5	15.8	17.3	17.3
M_4	U[0, 5]	5.1	5.1	0.2	0.2
X_5	U[0, 1]	59.9	60.7	66.4	66.4

Table 3. Results of sensitivity analysis of \overline{M}_{out} .

uncertainty model for M_2 upwards but keeping the same range of variation (i.e. from U[0, 5] to U[5, 10]), increases the influence of w_1 , whereas M_2 has the same influence as M_4 .

Note that the use of different spatial resolutions for the maps can influence the outcome of a sensitivity analysis. The whole exercise is repeated for 50×50 maps. These results are also shown in Tables 3–5. With the assumption of independence, a higher grid resolution produces more smoothing out of uncertainties, and consequently a reduction of the map's importance.

Table 4. Sensitivity analysis results where variability of w_1 has been altered.

Increase uncertainty of w_1				Lower value but same range of uncertainty of w ₁		
Variable	Pdf	Sobol' estimate of first-order sensitivity (%) 10 × 10	Sobol' estimate of first-order sensitivity (%) 50 × 50	Pdf	Sobol' estimate of first-order sensitivity (%) 10 × 10	Sobol' estimate of first-order sensitivity (%) 50 × 50
$\overline{w_1}$	U[0.4, 0.8]	41.5	45.0	U[0.2, 0.4]	15.5	16.4
M_2	U[0, 5]	3.3	0.2	U[0, 5]	1.4	0.1
w_3	U[0.5, 0.7]	10.3	8.6	U[0.5, 0.7]	15.6	16.7
M_4	U[0, 5]	3.4	3.4	U[0, 5]	5.4	0.3
X_5	U[0, 1]	40.7	36.6	U[0, 1]	62.0	67.5

Table 5. Sensitivity analysis results where variability of M_2 has been altered.

Increase uncertainty of M_2				Higher value but same range of uncertainty of M_2		
Variable	Pdf	Sobol' estimate of first-order sensitivity (%) 10 × 10	Sobol' estimate of first-order sensitivity (%) 50×50	Pdf	Sobol' estimate of first-order sensitivity (%) 10 × 10	Sobol' estimate of first-order sensitivity (%) 50 × 50
$\overline{w_1}$	U[0.5, 0.7]	60.1	64.3	U[0.5, 0.7]	36.4	44.3
M_2	U[5, 10]	2.8	0.1	U[0, 10]	14.8	0.8
w_3	U[0.5, 0.7]	6.7	7.1	U[0.5, 0.7]	8.5	10.9
M_4	U[0, 5]	2.5	0.1	U[0, 5]	3.4	0.2
X_5	U[0, 1]	26.9	28.6	U[0, 1]	36.7	43.3

These results show how it is important to undertake sensitivity analysis for even a simple model. In this example, the resolution of the input maps as well as the magnitude of uncertainty of each input can determine very different critical inputs.

4.2 Test example 2

A spatial model (AquiferSim) for simulating nitrate transport from paddock to aquifer was recently developed by Bidwell *et al.* (2005). Given the high levels of uncertainty in land-use and groundwater-flow information, it was appropriate for development purposes to do a preliminary SA to determine those inputs that had the most impact on model outputs. Uncertainty in six inputs was simulated: soil, land use, table of lookup values for nitrate and drainage (derived from a paddock-scale model), river recharge, aquifer porosity, and transmissivity (Table 6). This is an interesting example as it mixes spatial data, tabular data, and a constant. Autocorrelation was not simulated but could have been if information on spatial dependence of uncertainty had been available. The quasi-random sampling scheme was used to sample from the six pdfs with a sample size of 256. This required 3584 simulation runs, i.e. (2k+2)N runs, where k=6 and N=256. The objective function was chosen to be the maximum concentration of nitrate below a specific point location (site of a well).

To obtain empirical confidence intervals for the Sobol' indices, we have employed the bootstrap technique (Efron and Tibshirani 1993). At the given sample size selected for the experiment, 100 bootstrap replicas of the sample have been

Table 6. List of inputs to the AquiferSim model and the sensitivity analysis results.

Variable	pdf	First-order sensitivity index (90% confidence interval)	Total-effect sensitivity index (90% confidence interval)	Notes
Soil map	DU[0, 3]	13–30%	44–57%	Four alternative soil layers derived from a Monte Carlo simulation using a confusion matrix
Land-use map	DU[0, 3]	0–15%	12–24%	Four alternative layers derived from a Monte Carlo simulation using a confusion matrix
Nitrate/drainage table	DU[0, 1]	7–24%	12–18%	Two alternative tables of outputs from the paddock-scale model
River recharge map	DU[0, 1]	0–19%	18–35%	Two alternative maps – one with a constant value for each river, the other varies along each river
Aquifer transmissivity map	DU[0, 3]	9–30%	46–62%	Four alternative maps derived from expert judgement
Aquifer porosity	DU[0, 3]	0–0%	0–0%	Four alternative constant values (0.03, 0.1, 0.2, 0.3)

i=DU[a, b] is a discrete uniform distribution where an integer i is randomly selected with equal probability such that $a \le i \le b$.

obtained, providing 100 bootstrap estimates of the first-order and total-order indices. The 90% confidence intervals of these estimates are reported in Table 6. If smaller confidence interval of the sensitivity indices is required, then the sample size *N* should be increased.

The results from the spatial sensitivity analysis show that the soil and transmissivity layers are the most important inputs (Table 6). The sum of the first-order effects is only 55% indicating that there are significant effects (45% of the model output variance) due to interactions between the inputs. The transmissivity and river recharge maps are the most uncertain of the six layers, so these results indicate that more efforts should be devoted to improving the river flow model from which these two layers were derived. The results indicate that it may also be worthwhile to obtain better soil information, whereas aquifer porosity could be described by a constant.

5. Discussion

The advantages of the Sobol' (and extensions) method are that it (along with other methods based on the decomposition of variance) ensures that the entire model input space is explored, and it is a model-free sensitivity measure, which is independent of assumptions about the model structure. Other methods can be of limited use, if not outright misleading, when the analysis aims to assess the relative importance of model inputs (Saltelli *et al.* 2005).

In addition, this approach is able to distinguish between first-order effects and higher-order effects that account for interactions. Such information can be useful for purposes of model improvement, parameter estimation, or model simplification. Further, as shown by Tang *et al.* (2007b), the method yields more robust sensitivity rankings than other measures such as analysis of variance or regional sensitivity analysis. In this paper, we use equations (9)–(16), according to Tarantola *et al.* (2006b), which represent a further improvement of the accuracy of the Sobol' estimates.

Many of the SA techniques that have previously been applied to spatial data and models require that spatially variable inputs be reduced to a single scalar value. This severely constrains the ability to model spatial variability and structure. The approach presented here (like the winding stairs/Jansen approach) does not have this constraint. Geostatistical routines such as conditional sequential simulation (Pebesma and Wesseling 1998) allow spatial dependence to be simulated then analysed for its importance in a spatial model. This allows for realistic representations of spatial uncertainty that are auto-correlated as appropriate. Uncertainty in attribute value or location can be simulated, as well as spatial pattern, scale (or resolution), aggregation technique, or any combination of these. The method presented here can equally be used to assess the sensitivity of time-dependent input or even a spatial-temporal input. Furthermore, the relative effect of alternative sub-models versus uncertainty of spatial data can also be analysed by defining a SA input that selects between alternative sub-models or algorithms.

The approach presented in this paper should be applicable to all types of spatial models. In practice, the size of N depends on the computational cost of the model. Models that are expensive to run may constrain the analyst to select small N values (e.g. N=30-100), while cheap models can allow the analyst to use larger N values (e.g. N>500). Of course, for a given model, the larger the N, the more precise the sensitivity estimates. Complex non-linear models may require larger N values to achieve a given

accuracy for the sensitivity estimates. The approach presented here requires (2k+2)N simulations in order to calculate the sensitivity measures. This is considerably less than the $N \times N$ simulations required by a brute-force method (for which estimates of conditional expectations $E(Y|X_i=x_i^*)$ at a large number of x_i^* are required).

When simple random sampling is used to generate the spatial sample, N should be a multiple of each Nmaps_i, where Nmaps_i represents the number of map realisations for the ith (spatial) input, so that each map can be reused in the model a given number of times. For example, in a case with five spatial inputs, if we select $Nmaps_i = \{10, 15, 6, 12, 18\}$, the minimum usable value of N is 180. Of course 360, 540, and so on can also be used. With N=180, each realisation of the first map input would be used on average 18 times, the second map input 12 times, and so on. Note that the number of map realisations, Nmaps_i, should be sufficiently large to be representative of the uncertainty of each of the spatial inputs. In the particular case in which quasi-random sampling is employed to generate the spatial sample, each value of $Nmaps_i$ is constrained to be a power of 2, so that the sequence of quasirandom numbers can uniformly cover the input space. As an example, $Nmaps_i = \{16,$ 8, 64, 32, 8}, and the corresponding usable N value is 64, or 128, and so on. Given the potentially large data volume required to store multiple realisations of the spatial layers, it would be preferable to generate the necessary realisations only when they are needed, and delete them once the model has been run. However, in the case above where a given realisation has to be reused, it must be possible to replicate exactly the same realisation.

6. Conclusion

Of the various available sensitivity analysis techniques, only some are suited to spatial models. The Sobol' approach and its related extensions applied in a spatial context have some significant advantages: no assumptions are made about the model behaviour; first- and higher-order effects can be computed and analysed; the whole space of uncertain model inputs can be examined; a spatial layer can be treated as a random variable (allowing for the effect of spatial scale, structure, and autocorrelation to be analysed); and there are no constraints on how realisations of each spatial input are produced (allowing quite complex spatial descriptions of variability to be simulated). The applicability of the method of Sobol' in the presence of dependence among inputs has not been tested yet. The quasi-random sampling scheme can be used to reduce the number of simulations required to attain a given accuracy in the sensitivity estimates.

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