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Sensitivity analysis on spatial models: a new approach

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Abstract

Sensitivity analysis involves determining the contribution of individual input factors to uncertainty in model predictions. The most commonly used approach when doing a sensitivity analysis on spatial models is using Monte Carlo simulation. There are a number of techniques for calculating sensitivity indices from the Monte Carlo simulations, some more effective or efficient than others. These techniques are summarised along with their limitations. A new technique for undertaking a spatial sensitivity analysis based on the Sobol' method is proposed and tested. This method is global, variance-based, and model-free. The technique is illustrated with two simple test models.

Keywords: sensitivity analysis, uncertainty analysis, simulation, Monte Carlo

1 Introduction

Models of varying complexity are developed to approximate or mimic systems and processes in different aspects of the real world (e.g. physical, environmental, social, or economic). Applying models in the environmental domain inevitably involves uncertainty in both the model representation and in the input data.

Uncertainty analysis (UA) techniques can be applied to study uncertainty in model predictions arising from imprecisely known environmental processes and input data. Sensitivity analysis (SA) involves determining the contribution of individual input factors to the uncertainty in model predictions. Sensitivity analysis answers questions like 'which of the uncertain input factors is more important in determining the uncertainty in the output of interest?' Input factors can be poorly known model parameters (kinetic coefficients in chemical models, speed flows of radioactive species in the geosphere, etc.), errors in input data, and also more complex entities such as alternative sub-models, flow fields, the use of one mesh size rather than another.

There are a variety of SA techniques that can be employed, most of which involve multiple simulations of the model of interest. This approach has been used many times with single-dimensional models and time-series models but more rarely with spatial models. This is because the multi-dimensionality of spatial models can make doing an SA quite onerous. Indeed, some of the methods simply aren't practical, while others have significant limitations. Simulation approaches that have been applied to spatial problems are described in the next section.

2 Background

The one-at-a-time (OAT) approach is the most common method, in which only 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 and 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 (Lodwick *et al*., 1990) in that the other parameters are not varied but fixed at nominal values, so the SA is limited to a small area of the parameter space. Because of this SA results may not be generally valid. Furthermore, OAT can only examine first-order effects; interactions between parameters cannot be detected. The analysis tends to be relatively informal and *ad hoc*. Error is generally modelled as a scalar, e.g. increasing rainfall by a fixed amount.

Another approach is to simplify the spatial dimension by reducing the spatial variability to just a few zones, each of which is treated as a random variable (RV). Hall *et al*. (2005) use 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 RV parameters. Each region can be correlated to an adjacent region. In this case, global SA techniques can be used (where all inputs are varied simultaneously). This approach is only suitable if the number of spatial regions with different values is very small.

A variation of this spatial simplification approach is to randomly or purposefully select a small representative set of pixels or points, and either do an SA on each or combine into one large SA, e.g. Avissar (1995), Dubus and Brown (2002), Lilburne *et al*. (2003). This approach is only suitable where the model can be treated as an aspatial model run at various points in the landscape.

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 the input *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). However, this approach is computationally very inefficient, although computation could be reduced through judicious grouping of input sources such that each group is kept constant in turn. Note that it is possible for the variance due to input *i* to increase (relative to total variance) rather than decrease in cases where the error is biased (Saltelli *et al*., 2004), which confuses interpretation of results.

All of the approaches described above have significant limitations. Ideally a spatial SA should combine a full global SA (in which all inputs of interest are varied simultaneously and efficiently), with the ability to generate autocorrelated realisations of the input map RVs. The SA technique should then work on the input map as a whole rather than individual pixels or polygons, thus allowing the spatial structure to be included in the analysis. This excludes regression and FAST techniques, as they require scalar input values.

The winding stairs/Jansen technique (Jansen *et al*., 1994) has been successfully applied by Kros *et al*. (1999) thus achieving a global spatial SA. In this paper the Sobol' technique (Sobol', 1993) is applied to spatial input data, which has not to our knowledge been done before.

3 Sensitivity Analysis techniques

There are many techniques for SA including linear regression or correlation analysis, measures of importance, sensitivity indices, screening, etc. (Saltelli *et al*., 2000; Helton, 1993). In this paper we focus on variance-based measures, which are now described.

Let us assume that the computational model is given by $Y = f(X_1, X_2, \ldots, X_k)$, where X_i are independent input variables, and Y is the model output. When using variance-based techniques (Archer *et al*., 1997), f can be either linear, non linear, additive or non additive, and SA estimates the fractional contribution of each input variable X_i to the variance of Y. In order to calculate the sensitivity indices for a set of independent X_i, the total variance $V(Y)$ of the model output is decomposed as:

$$V = \sum_i V_i + \sum_{i<j} V_{ij} + \sum_{i<j<m} V_{ijm} + \ldots + V_{12\ldots k} \tag{1}$$

where

$$V_i = V(E(Y|X_i)) \tag{2}$$

$$V_{ij} = V(E(Y|X_i, X_j)) - V_i - V_j \tag{3}$$

and so on. Equation (1) contains ${}^kC_1 = k$ first-order terms, ${}^kC_2 = ½\ k\ (k - 1)$ second-order terms, and so on with a total of $\sum({}^kC_1 + {}^kC_2 + \ldots + {}^kC_k) = 2^k - 1$ terms. The second-order terms V_{ij} capture the interaction effect between X_i and X_j. $E(Y \mid X_i = x_i^*)$ denotes the expectation of Y conditional on X_i having a fixed value x_i^*. The generic sensitivity index of order s is defined as:

$$S_{i_1, i_2, \ldots, i_s} = \frac{V_{i_1, i_2, \ldots, i_s}}{V} \tag{4}$$

where i_1, i_2 etc refer to the input factors. For example, S_i for the factor X_i is defined as V_i / V. The reason for that is intuitive: if the inner mean $E(Y \mid X_i = x_i^*)$ for some particular value $X_i = x_i^*$ varies considerably with respect to the total variance, while all the effects of the X_j's, $j \neq i$ are being averaged, then surely factor X_i is an influential one. Similarly, S_{12} is the pure interaction effect between X_1 and X_2, i.e. that part of the variation in Y due to X_1 and X_2 which cannot be explained by the sum of the individual effects of X_1 and X_2, and so on.

Estimation procedures for S_i are the Fourier Amplitude Sensitivity Test (FAST) (Cukier *et al*., 1973), the extended FAST (Saltelli *et al*., 1999), the High Dimensional Model Representations (Rabitz and Alis, 2000), the method of Sobol' (1993), and its improved versions (Tarantola *et al*., in press, Saltelli, 2002). Variance-based methods display a number of attractive features for SA:

- model independence: the sensitivity measure is model free
- captures the influence of the full range of variation of each variable
- captures interaction effects; this can be a crucial issue for a design problem, or for a risk analysis study
- SA can be performed on subgroups of input variables; in complex models uncertain variables might pertain to different logical levels, and it might be desirable to decompose the uncertainty according to these levels.

3.1 The Sobol' method

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

- Choose a base sample dimension *N*.
- Generate a Monte Carlo sample of the input factors (dimension 2*N*) and define two matrices of data (*A* and *B*), each containing half of the sample (ordered by column).
- Define a matrix Di formed by all columns of A, except the i-th column, which is taken from B and a matrix Ci formed with the i-th column of A and with all the remaining columns of B (Figure 1).

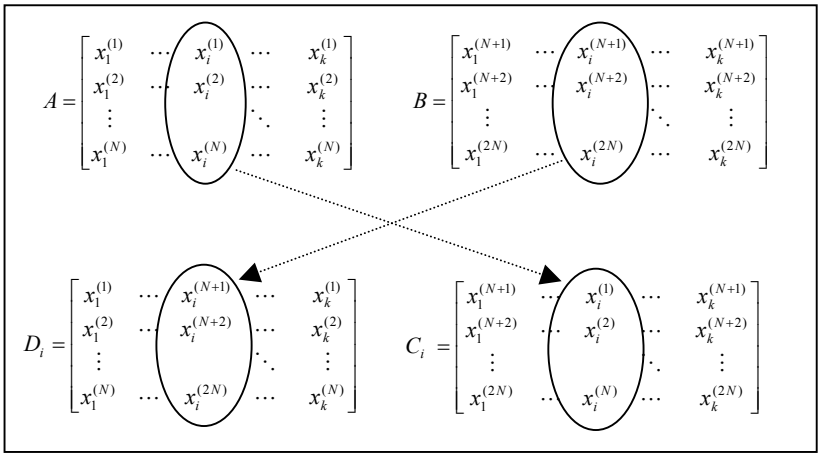

Figure 2 Generating matrices Ci and Di from A and B.

Compute the model output for all the input values in the sample matrices *A*, *B*, C_i and D_i, obtaining four vectors of model outputs of dimension $N \times 1$:

$$\mathbf{y}_A = f(A), \mathbf{y}_B = f(B), \ \mathbf{y}_{C_i} = f(C_i), \ \mathbf{y}_{D_i} = f(D_i) \tag{5}$$

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

$$S_i = \frac{V_i}{V} = \frac{V_{X_i}[E_{\mathbf{X}_{-i}}(Y \mid X_i)]}{V} = \frac{\mathbf{y}_A \cdot \mathbf{y}_{C_i} - f_0^2}{\mathbf{y}_A \cdot \mathbf{y}_A - f_0^2} = \frac{\frac{1}{N}\sum_{j=1}^{N} y_A{}^{(j)} y_{C_i}{}^{(j)} - f_0^2}{\frac{1}{N}\sum_{j=1}^{N} (y_A{}^{(j)})^2 - f_0^2} \tag{6}$$

where:

$$f_0^2 = \left(\frac{1}{N} \sum_{j=1}^{N} y_A^{(j)} \right)^2 \text{ (the mean), and} \quad (7)$$

$E_{X\text{-}i}$ is the expected value obtained by considering all factors except X_i.

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

$$S_{Ti} = 1 - \frac{V_{-i}}{V} = 1 - \frac{V_{\mathbf{X}_{-i}}[E_{X_i}(Y \mid \mathbf{X}_{-i})]}{V} = 1 - \frac{\mathbf{y}_A \cdot \mathbf{y}_{D_i} - f_0^2}{\mathbf{y}_A \cdot \mathbf{y}_A - f_0^2} = 1 - \frac{\frac{1}{N}\sum_{j=1}^{N} y_A^{(j)} y_{D_i}^{(j)} - f_0^2}{\frac{1}{N}\sum_{j=1}^{N} (y_A^{(j)})^2 - f_0^2} \quad (8)$$

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

In this work, we will use a generalisation of formulas 6 and 8, described in Tarantola *et al*. (in press). Symmetries and dualities of the estimation formulas are explored and, at no extra sampling (i.e. no further model simulations), we can obtain additional estimates of first-order and total-effect sensitivity indices. When we estimate V_i as sum of products $y_A\, y_{Ci}$, it is better to estimate f_0^2 using products of independent vectors y_A and y_B (rather than using y_A only):

$$f_0^2 = \frac{1}{N^2} \sum_{j=1}^{N} y_A^{(j)} \sum_{j=1}^{N} y_B^{(j)} \quad (9)$$

Besides, it is also legitimate to estimate f_0^2 using products of vectors y_{Ci} and y_{Di}, which are also independent (the estimate of f_0^2 depends on i in such case):

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

When equation 9 is employed, the total-output variance V can then be calculated from either $y_A\, y_A$ or $y_B\, y_B$. Similarly, when we estimate f_0^2 using equation 10, the variance can be estimated from either $y_{Ci} y_{Ci}$ or $y_{Di} y_{Di}$. We end up with four sensitivity indices:

$$S_i^I = \left(\sum y_A y_C - \sum y_A y_B\right) / \left(\sum y_A y_A - \sum y_A y_B\right) \quad (11)$$

$$S_i^{II} = \left(\sum y_A y_C - \sum y_A y_B\right) / \left(\sum y_B y_B - \sum y_A y_B\right) \quad (12)$$

$$S_i^{III} = \left(\sum y_A y_C - \sum y_C y_D\right) / \left(\sum y_C y_C - \sum y_C y_D\right) \quad (13)$$

$$S_i^{IV} = \left(\sum y_A y_C - \sum y_C y_D\right) / \left(\sum y_D y_D - \sum y_C y_D\right). \quad (14)$$

Further, exploiting the symmetry property of equation 6, we obtain four additional indices:

$$S_i^V = \left(\sum y_B y_D - \sum y_A y_B\right) / \left(\sum y_A y_A - \sum y_A y_B\right) \quad (15)$$

$$S_i^{VI} = \left(\sum y_B y_D - \sum y_A y_B\right) / \left(\sum y_B y_B - \sum y_A y_B\right) \quad (16)$$

$$S_i^{VII} = \left(\sum y_B y_D - \sum y_C y_D\right) / \left(\sum y_C y_C - \sum y_C y_D\right) \quad (17)$$

$$S_i^{VIII} = \left(\sum y_B y_D - \sum y_C y_D\right) / \left(\sum y_D y_D - \sum y_C y_D\right) \quad (18)$$

The mean value of these eight sensitivity indices S_i^I, S_i^{II}, S_i^{III}, S_i^{IV} S_i^V, S_i^{VI}, S_i^{VII}, and S_i^{VIII} yields more accurate estimates instead of just using equations 6 and 8, for which we would need much larger N to achieve the same level of accuracy. Using the same symmetry properties we can estimate four total-sensitivity indices.

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

4 Application of Sobol' technique to spatial models

4.1 Test example 1

A simple model is used to demonstrate this approach to SA. The model is a weighted composite index:

$$Index = \sum_{i=1}^{n} w_i X_i \quad (19)$$

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 spatially 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 of output map M_{out} where

$$M_{out} = w_1 M_2 + w_3 M_4 + X_5 \quad (20)$$

M_2 and M_4 are input maps, X_5 is a scalar input, and w_1 and w_3 are weights. The uncertainty of each independent and uncorrelated input is shown in Table 1.

Results depend on the scale of the map. For a map of 10×10 pixels, Table 1 shows that X_5 is the most sensitive input given the specified ranges of uncertainty. If the uncertainty of the weights is increased, then their sensitivity increases as expected (not shown). If the range of uncertainty in a map increases then sensitivity to the map will increase as expected (M_2 in Table 2). However, if range shifts rather than increases, map sensitivity does not change (not shown).

For a 50×50 map however, the sensitivity of the maps is quite low. This is because as the number of pixels or random values increases, their expected mean will stabilise. In other words, no matter how big the uncertainty of individual pixels or polygons, averaging them will smooth or minimise the impact of this uncertainty.

Table 1 Results of sensitivity analysis of M_{out}.

Variable	PDF	Sobol' estimate of sensitivity (%) 10×10	Sobol' estimate of sensitivity (%) 50×50
w1	U[-0.5, 0.5]	12.5	16.4

M2	U[-5, 5]	13.1	0.8
w3	U[-0.5, 0.5]	12.7	16.4
M4	U[-5, 5]	12.8	1.2
X5	U[-1, 1]	50	66

Table 2 Sensitivity analysis results where variability of M2 has been increased.

Variable	PDF	Sobol' estimate of sensitivity (%) 10×10	Sobol' estimate of sensitivity (%) 50×50
w1	U[-0.5, 0.5]	9.1	15.9
M2	U[-10, 10]	37.2	2.8
w3	U[-0.5, 0.5]	9.3	16.3
M4	U[-5, 5]	9.4	1.1
X5	U[-1, 1]	36.4	65

4.2 Test example 2

The Structural Vulnerability Index (SVI) estimates the inherent susceptibility of New Zealand soils to physical degradation from intensive cultivation or grazing (Hewitt and Shepherd, 1997). It is calculated from four soil properties (phosphate retention (%), total organic carbon (%), clay content (%), and drainage class). The index ranges from 0 to 100 (low – high vulnerability). The likely range of each of these variables is described in a soil spatial database, the Fundamental Soil Layers (Wilde *et al*., 2000). Using this information, two approaches were used to generate 100 realisations of each property for the area of interest. The first was simple random simulation using a uniform distribution between the minimum and maximum values. The second was to model and simulate variability using the geostatistical technique of unconditional sequential simulation (Pebesma and Wesseling, 1998). Figure 2 shows an auto-correlated realisation of carbon. The objective function of interest (i.e. *Y*) is the proportion of the area that is classified as having very low vulnerability (svi < 35).

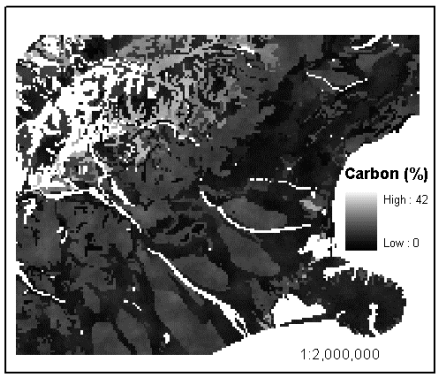

Figure 2 A realisation of carbon generated by GSTAT.

The Sobol' preprocessor generated matrices A and B (with $k = 4$, $N = 200$) by associating a spatial realisation with the scalar value sampled from a discrete U[1,100] distribution. If the same scalar value is sampled twice from the distribution, we must feed the model with the same realisation.

Each matrix element references one of the 400 spatial realisations. The GIS was programmed to run the model $(2k+2)N$ times generating four vectors (equation 5). The postprocessor then calculated the sensitivity measures (Table 3).

Table 3 Results of SA on SVI model using Sobol' technique.

Input variable	S_i	S_{Ti}
Drainage	0	0.05
P retention	0.12	0.34
Carbon	0.46	0.53
Clay	0.18	0.3

The area of very low structural vulnerability is most sensitive to the carbon layer and least sensitive to the drainage class. The sum of first-order indices is 0.76, meaning that 24% of the output variance is accounted for by higher-order interactions. The total-effect index which accounts for these interactions shows that 53% of the variability is due to the carbon layer.

5 Discussion

The advantage of the method of Sobol', and in general of all the methods based on the decomposition of the model output variance, is that 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 input factors (Saltelli *et al*., 2005). The calculated estimates of sensitivity distinguish between first-order effects, and higher order effects which account for interactions. If first-order effects dominate then resources can be focused on improving the most sensitive input(s). If higher-order effects dominate then care should be taken to characterise interactions between variables.

Another important advantage of the Sobol' method in a spatial context is that, unlike most other SA methods, it lends itself to the use of geostatistical techniques for generating alternative realisations of spatial inputs. This allows for realistic representations of spatial uncertainty that are autocorrelated 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. This method can equally be used to assess the sensitivity of a time series or even a spatio-temporal input, as well as scalars and spatial inputs. All that is needed is a method for randomly generating alternative realisations for each input.

Given the potential size requirements of multiple realisations of the spatial layers, it is desirable to generate the necessary realisations only when they are needed, and deleting them once the model has been run. However, the Sobol' preprocessing technique involves reusing some of the realisations. Either all the realisations must be stored before running the model or it must be possible to regenerate a given realisation by specifying its seed. In the two test examples above, all the realisations were created beforehand.

As a general rule of thumb N should be in the order of some hundred. More complex or irregularly behaved models may require more simulations. The Sobol' 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.

If the layers contain many map units or pixels, the model does not depend on spatial structure, and the objective function is a mean, then spatial variation will tend to average out and the corresponding uncertainty of Y may become smaller. Simulating spatial autocorrelation and between-layer correlation (if present) is important for gaining a useful understanding of variation in the output. Currently the Sobol' technique requires that the X_i are independent. However, work is underway to extend the method to cater for correlated inputs.

6 Conclusions

A new approach to doing a global SA on a spatial model has been presented and tested on two simple examples. The approach is based on the Sobol' technique, which is independent of any model of the variability, is a global technique, and is derived from decomposition of variance. An important advantage of applying this technique to the SA of a spatial model is that there are no constraints on how the realisations of each input variable are produced, which means that quite complex spatial descriptions of variability can be simulated. An algorithmic extension to the Sobol' technique that makes the approach more efficient, was also described. This new SA approach is promising and will be applied in a more challenging spatial-modelling case study.

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