Environmental Modelling & Software 26 (2011) 723–730

Contents lists available at ScienceDirect

Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft

Variance-based sensitivity analysis of model outputs using surrogate models

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ARTICLE INFO

Article history:
Received 29 October 2009
Received in revised form
27 December 2010
Accepted 4 January 2011
Available online 5 February 2011

Keywords:
Sensitivity analysis
Surrogate models
Experimental design
Computational cost

ABSTRACT

If a computer model is run many times with different inputs, the results obtained can often be used to derive a computationally cheaper approximation, or surrogate model, of the original computer code. Thereafter, the surrogate model can be employed to reduce the computational cost of a variance-based sensitivity analysis (VBSA) of the model output. Here, we draw attention to a procedure in which an adaptive sequential design is employed to derive surrogate models and estimate sensitivity indices for different sub-groups of inputs. The results of such group-wise VBSAs are then used to select inputs for a final VBSA. Our procedure is particularly useful when there is little prior knowledge about the response surface and the aim is to explore both the global variability and local nonlinear features of the model output. Our conclusions are based on computer experiments involving the process-based river basin model INCA-N, in which outputs like the average annual riverine load of nitrogen can be regarded as functions of 19 model parameters.

1. Introduction

The purpose of variance-based sensitivity analysis (VBSA) is to provide a better understanding of the output of complex computer models (Saltelli et al., 2004). More specifically, the aim is to apportion the total variability of the model output to the variability or uncertainty of various inputs. Due to the rapid progress of computer technologies, VBSA is increasingly utilized in many fields of science. However, it is not unusual that the computational cost becomes insurmountable, because such analyses may require a very large number of model runs. This has prompted several scientists to investigate whether the computational cost can be reduced by performing the VBSA on a computationally cheaper surrogate model of the original computer code. Li and co-workers (2002, 2006) considered truncated high-dimensional model representation (HDMR) expansions of the original model. Oakley and O'Hagan (2004) used a Gaussian emulator, and Ratto et al. (2006) employed state-dependent parameter modeling. Storlie and Helton (2007) and Storlie et al. (2009) examined how a variety of regression smoothers can facilitate VBSA. Busby (2009) developed a sequential adaptive design of experiment to obtain a Gaussian emulator using the least possible number of function evaluation. Sudret (2008) proposed a substitute analytical form for Sobol' indices using generalized polynomial chaos expansions (PCE), and could reduce the computational cost of the sensitivity indices by estimating the PCE coefficients.

VBSA provides information about the sources of the total variability of the model output over the entire input domain. Our goal was to investigate how VBSA based on surrogate models can be integrated with techniques that give more detailed information about the variability of the model output. In particular, we examined how we could perform a VBSA and at the same time identify subregions of the input domain where the model output is strongly nonlinear.

Our approach is based on a sequential adaptive design algorithm that was developed to enable accurate prediction of the model output at untried inputs even when the curvature of the model output varies strongly over the input space (Shahsavani and Grimvall, 2009). We used the river basin model INCA-N (Wade et al., 2002) as a study object to illustrate how the mentioned design algorithm can be combined with a simple grouping of the model inputs to facilitate handling of relatively high-dimensional inputs. Furthermore, we demonstrated how simple summaries of the distribution of design points can provide information about subregions with a strongly nonlinear response.

2. The INCA-N model

INCA-N is a semi-distributed, process-based deterministic model of the flow of water and nitrogen through catchments (Whitehead et al., 1998a,b; Wade et al., 2002). It simulates the key

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doi:10.1016/j.envsoft.2011.01.002

factors and processes that affect the amount of NO_3 and NH_4 stored in the soil and groundwater systems, and it feeds the outputs from these systems into a multi-reach river model. The inputs to the INCA-N model represent natural (meteorological) forcing, anthropogenic forcing (fertilization schemes), and a set of model parameters. The outputs comprise daily estimates of water flow and NO_3 and NH_4 concentrations in stream water at discrete points along the main channel of the river (Fig. 1). We focused on a derived output: the average annual riverine load of inorganic nitrogen over a period of seven years where the output at each time point is represented by the product flow $\times$(No_3–N + NH_4-n). Furthermore, we restricted our analysis to an artificial model catchment consisting of a single sub-basin covering 1 km^2 of agricultural land. Meteorological inputs, fertilization schemes, and model parameters were taken from a case study of the Tweed river basin in Scotland and England. The input parameters of the INCA-N model can be divided into three major groups:

- *Initial states of the river basin*;
- *Nitrogen transformation parameters* that refer to the rates at which nitrogen is transformed in the soil or via take up by crops;
- *Hydrogeological parameters* that control the properties of water in the soil.

Table 1 summarizes the dimension and range of those inputs in our study.

3. Construction of surrogate models

Let a computer code model with inputs in a cuboid $D = \{x;\ a_j \le x_j \le b_j,\ j = 1,\ldots,p\}$ be analytically expressed by $y = f(x_1,\ldots,x_p)$. The construction of surrogate models of such functions was based on our developed methodology (Shahsavani and Grimvall, 2009), which includes two steps:

- sequential, adaptive selection of the design points at which the investigated model is run;
- prediction of model outputs at untried inputs by local fitting of quadratic polynomials to the model outputs already computed in cautiously selected neighbourhoods of the query points.

The design algorithm started by taking the centre and corners of input domain and centre points of $p-1$ non-opposite faces of this cuboid. Thereafter, the input domain D was successively split into disjoint cuboids whose corners and centre point were incorporated into the design. In each step, it was needed to determine which cuboid had to be split into two halves, and along which axis the cut had to be made. Thus, measures of nonlinearity or roughness of the

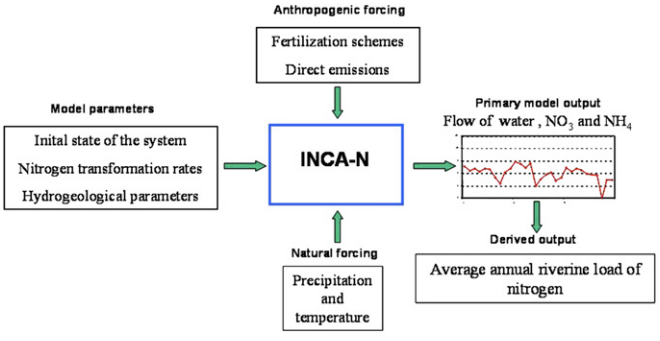

Fig. 1. Structure of the process-based INCA-N model of the flow of nitrogen and water through a river basin.

Table 1
Model parameters in the INCA-N model.

Group	Variable name	Unit	Range
Initial conditions	Surface flow	m^3/s	[0, 0.01][a]
	Surface nitrate	mg N/l	[0, 10]
	Surface ammonium	mg N/l	[0, 2]
	Surface drainage volume	m^3	[10^5, 2×10^7][a]
	Sub-surface flow	m^3/s	[0,0.01][a]
	Sub-surface nitrate	mg N/l	[0,10]
	Sub-surface ammonium	mg N/l	[0,2]
	Sub-surface drainage volume	m^3	[10^5, 2×10^7][a]
Nitrogen transformation (rate)	Denitrification	mol/day	[0, 0.01]
	Nitrogen fixation	kg N/ha/day	[0, 0.01]
	Plant nitrate uptake	mol/day	[0, 0.05]
	Maximum nitrate uptake	kg N/ha/yr	[80, 140]
	Mineralization	kg N/ha/day	[0, 1]
	Immobilization	mol/day	[0, 0.1]
	Plant ammonium uptake	mol/day	[0, 0.05]
Hydrogeological parameters	Soil moisture deficit	mm	[100, 170]
	Soil water residence time	day	[0.5, 5]
	Groundwater residence time	day	[10, 200]
	Maximum soil retention volume	m	[0.1, 1]

[a] The range refers to an artificial study area consisting of 1 km^2 of agricultural land.

response in each of the current cuboids were computed to ensure that the splitting was directed towards cuboids in which the response was difficult to predict. The measure of nonlinearity of the response surface in a cuboid D^* was based on to the roughness measure

$$R\left(D^*\right) = \int\cdots\int_{D^*}\left(\sum_{i=1}^{p}\left(\frac{\partial^2 f}{\partial x_i^2}\right)^2 + 2\sum_{i<j}^{p}\left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)^2\right)\mathrm{d}x_1\mathrm{d}x_2\cdots\mathrm{d}x_p$$

(Green and Silverman, 1994).

The measure of roughness assigned to a cuboid D^* was determined by fitting a second order polynomial

$$P_{D^*} = \alpha_0 + \sum_{j=1}^{p}\alpha_j x_j + \sum_{j=1}^{p}\beta_j x_j^2 + \sum_{j<k}\gamma_{jk}x_j x_k$$

to design points inside, on, or close to the border of D^* and then computing

$$\widehat{R}\left(D^*\right) = V\left(D^*\right)\left(\sum_j\left(2\widehat{\beta}_j d_j^2\right)^2 + 2\sum_{j<k}\left(\widehat{\gamma}_{jk}d_j d_k\right)^2\right)$$

where $V(D^*)$ denotes the volume of D^* and d_j depicts the length of the jth side of D^*. Furthermore, the cuboid with the largest roughness index was split along the axis for which

$$\tilde{S}(j) = \left|\widehat{\beta}_j\right| d_j^2$$

attained its maximum.

The above mentioned structure provided designs that were space filling and comparatively dense in those parts of the input domain where the response was more nonlinear, whereas other parts of the input domain were more sparsely covered. In fact the algorithm was designed so that it could distinguish a cuboid with higher roughness in each step and then generate the design points in this cuboid. It means that practically the cuboids with less roughness measures have fewer design points. Hence, it can be expected that the input domain is sparsely covered where the relationship between input and output is almost flat.