Environmental Modelling & Software 69 (2015) 166–174

Contents lists available at ScienceDirect

Environmental Modelling & Software

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

Introductory Overview

An introduction to sensitivity assessment of simulation models☆

John Norton [a, b, *]

[a] Integrated Catchment Assessment & Management, Fenner School of Environment & Society, The Australian National University, Canberra, ACT 2601, Australia
[b] School of Electronic, Electrical & Systems Engineering, University of Birmingham, Birmingham B15 2TT, UK

ARTICLE INFO

Article history:
Received 6 August 2014
Received in revised form
27 March 2015
Accepted 29 March 2015
Available online 15 April 2015

Keywords:
Overview
Sensitivity analysis
Simulation models
Algebraic sensitivity analysis
Sensitivity index
Emulators

ABSTRACT

In view of increasing application of sensitivity assessment (SA) to environmental simulation models, a relatively short, informal introduction to aims and methods of SA is given. Their variety, motivation and scope are illustrated by outlines of a broad selection of approaches. Methods based on derivatives, algebraic analysis, sparse sampling, variance decomposition, Fourier analysis and binary classification are included.

1. Objective

This paper is an informal, selective guide to aims and methods of sensitivity assessment (SA) for simulation models. The selection is intended to be representative but isn't claimed to be comprehensive. However, some topics which seldom get attention will be discussed, for instance algebraic SA in Section 3.3 and regionalised SA in Section 3.5.6. More detail can be found via the references.

The paper is motivated by increasing and now widespread recognition of two facts. The first is that an environmental (or any other) simulation model's credibility and utility depend on knowledge of how important each parameter is; without SA and some idea of the quality of the model's structure and parameter estimates, we don't know how far to trust any prediction by the model. The second is that the results of SA show where the model needs improvement. The more important parameters may need refinement. Conversely, parts with little influence on the outputs of interest are poorly determined in calibration by those outputs; they should be simplified or removed to leave a model well justified by the data.

2. What is sensitivity assessment?

SA investigates the relations between parameters and outputs of a simulation model. In this context "parameters" are primarily equation coefficients and threshold values in the model, but may also include features of input (forcing) variables, *e.g.* their values if constant, or the time, duration, location, spatial extent or rate of any changes. [Parameters are often called "factors" in SA, and occasionally "inputs", which is confusing]. An "output" is the value of any variable computed by the model or of any feature or statistic extracted from it, such as peak or mean value. The supposition is that each parameter and output can be described by a single number. This is appealingly simple and allows SA to be thought of as examining the shape of the response surface of each output to the parameters. It's also restrictive, of course, and may not be tenable if, in particular, the model has dynamics. In that case, an output depends at any instant on the history of the inputs, which would take a very large (theoretically infinite) number of values to describe fully. What's more, we may well be interested in the whole response to the forcing, measured at a large number of instants. Models with dynamics are considered in Section 3.4.

SA tries to answer such questions as:

- For each output, in what order of importance do the parameters influence it?

☆ Introductory Overviews provide concise overviews on essential modelling concepts, with the aim of breaking down barriers to shared understanding and dialogue within multidisciplinary teams. See the Editorial in Vol 47 (Sept 2013) for more information.

* Integrated Catchment Assessment & Management, Fenner School of Environment & Society, The Australian National University. Tel.: +61 2 6295 7073, +33 497 021267.
E-mail address: john.norton@cantab.net.

http://dx.doi.org/10.1016/j.envsoft.2015.03.020
1364-8152/

- Are there parameters which affect the outputs so little that the model should be rewritten without them?
- How well can the combined effect of a collection of parameters be found by summing their individual effects?
- Conversely, what are the significant interactions between parameters in their effect on an output?
- How closely is an output change proportional to the change in parameter value which causes it?
- More broadly, how does the effect of a given change in a parameter value vary with that value?

These questions need not involve uncertainty, so SA is not the same thing as uncertainty assessment (UA). UA is in effect SA together with a specification of parameter uncertainties. The two get conflated because SA is often done by looking at the output values due to samples from a given distribution of parameter values, as in most of the methods described in Section 3.5. In any case, some specification of parameter uncertainty, even if only guessed ranges, is needed to define the scope of all but the most narrowly focused SA.

It isn't uncommon to find UA unaccompanied by SA. In most of the system identification literature (Norton, 1986; Walter and Pronzato, 1997; Ljung, 1999), parameter-estimation techniques provide estimates of parameter uncertainty (e.g. covariance) yet rarely try to analyse the sensitivity of the model outputs to those parameters.

This paper calls *SA sensitivity **assessment** rather than analysis*, as it is much more often done by numerical experiment, looking at the results of model runs, than by analysis of the model's equations. That said, such analysis may be possible if the model isn't too elaborate: see Sections 3.3 and 3.4.

3. SA techniques

3.1. Introduction

3.1.1. Assumed mathematical background

To see how any SA technique works, what assumptions it makes, what its scope and limitations are and what its results say, a little mathematics is needed. Only the bare essentials will be used here: basic calculus, the idea that a collection of items (model parameters, usually) can be viewed as a vector in a space with one axis per item, and the concepts of probability density and expectation.

3.1.2. Notation

In what follows, p denotes parameter and y output; δ means "change in", so δp is change in p, not necessarily small. A collection such as m parameters $p_1, p_2,\ldots, p_m$, indexed by a subscript, may be written as a single entity in boldface, e.g. $\mathbf{p}$ is the vector of elements $p_1, p_2,\ldots, p_m$ (in a column, by convention). The rate of change $\partial y/\partial p$ of a single output y with a single parameter p may be approximated, in practice, by $\delta y/\delta p$ where δy is the change in y caused by a finite change δp. When two parameters p_j and p_k have interacting effects on y, the rate of change of $\partial y/\partial p_j$ with p_k or of $\partial y/\partial p_k$ with p_j is $\partial^2 y/\partial p_j \partial p_k$, approximated by $\delta(\delta y/\delta p_j)/\delta p_k$.

Additive effects or components will be written out fully as summations rather than more concisely as vector inner products. For example, if interactions can be ignored and the parameter-to-output relations are smooth, the effect of small changes δp_1 to δp_m on y is approximated by $\delta y \cong \sum_{j=1}^{m} \frac{\partial y}{\partial p_j}\delta p_j$.

3.1.3. Motivation of SA techniques

There are a large number of SA techniques: ways to vary parameter values and examine their effects on the outputs. One might well ask why there are so many, when all you need to do, apparently, is try a lot of parameter values in succession and record the output values. The answer is that unless you are only interested in variation of a few parameters at once, over small ranges, it would take an enormous number of model runs to explore the parameter-output relations thoroughly. For example, to cover all combinations of only 5 values each of 10 parameters, 5^{10} simulation runs are needed. At, say, 1 s per run that would take over 16 weeks. We must be much more economical. Another factor, seldom given due weight, is the difficulty of making sense of a huge volume of sensitivity results. Again we have to be selective. Two possibilities are to examine results from a relatively small set of parameter and output samples, in the hope that they are representative, or to analyse the model algebraically. Where it can be done, algebraic analysis is likely to give more insight than a heap of numbers from many model runs. Another way to keep the volume of results manageable is to compute sensitivities as quantities averaged over the whole credible range of the parameters. This is called global SA, in contrast to local SA of sensitivities at particular parameter values.

We start with the simplest (and most naïve) technique and go on to methods which require more thought but yield a great deal of useful information while being economical in computing.

3.2. One-at-a-time perturbations

The simplest idea is to perturb one parameter at a time and see how much the output changes. For now, think about a change from p_j to $p_j + \delta p_j$ in one parameter, causing a change in a particular single-number output from y_i to $y_i + \delta y_i$. [Section 3.4 will look at time-varying outputs]. Although $\delta y_i/\delta p_j$ says something about how sensitive y_i is to p_j alone, it has three limitations: (i) it may vary with the size of δp_j, i.e. the cause-effect relation may not be linear, (ii) it may vary with other parameters, i.e. there may be interaction, and (iii) it depends on the units employed for δp_j and δy_i. We can get rid of this dependence by expressing the changes as *proportions* $\delta p_j/p_j$ and $\delta y_i/y_i$ and the result as the *normalised sensitivity* $\frac{\delta y_i/y_i}{\delta p_j/p_j} = \frac{p_j}{y_i}\frac{\delta y_i}{\delta p_j}$. Alternatively, if we knew the uncertainty in each parameter, we could express a change in a parameter value in terms of its standard deviation or range of uncertainty. To avoid specifying the size of δp_j, the sensitivity is formally defined through the rate of change $\lim_{\delta p_j \to 0} \delta y_i/\delta p_j = \partial y_i/\partial p_j$ approached as the parameter change is made ever smaller, giving normalised sensitivity $s_{ij} \equiv \frac{p_j}{y_i}\frac{\partial y_i}{\partial p_j}$. Its value is generally valid only at whatever values p_j and the other parameters have, and relates only to changes in p_j small enough for any non-linearity in the p_j-to-y_i relation to be ignored. Normalisation might be objected to on the grounds that when the relation is a straight line not through the origin, it turns a constant sensitivity into one which varies with p_j. That's true, but on the other hand one may well prefer to think of changes, errors and uncertainties as proportions (or percentages) rather than absolute values.

Although defined for infinitesimal changes, s_{ij} is estimated from the result of a finite parameter change: with all the parameters set to selected values, run the model and note y_i, change p_j alone by a chosen amount δp_j and rerun the model, note δy_i and get s_{ij} roughly as $\widehat{s}_{ij} = \frac{p_j}{y_i}\frac{\delta y_i}{\delta p_j}$. Perturbing m parameters in turn, all from the same start, will take $m+1$ runs.

The first problem in this seemingly straightforward method is to decide on the size of δp_j: small enough for $\widehat{s}_{ij}$ to be close to s_{ij}, or big enough to show the effect of realistic uncertainty in p_j? A small parameter change has two potential snags. The first is doubt over how linear the model is, and thus whether the result of a small change is a useful guide to the effects of larger changes. Second, calculation of $\widehat{s}_{ij}$ may be ill conditioned, with δy_i a small difference of large quantities. For these reasons we might prefer a larger