A Parameter-Bounding Approach to Sensitivity Assessment of Large Simulation Models

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EXTENDED ABSTRACT

Traditional sensitivity assessment (SA) methods have limitations which motivate a new approach, the subject of a new project at ANU and the Universities of Adelaide and Melbourne, with the Murray-Darling Basin Commission and the South Australia Dept. of Water, Land and Biodiversity Conservation as partners. The limitations include high computing load, restricted scope and validity of the results, excessive volume of results and failure to distinguish SA from uncertainty assessment. The new approach has three main aims: (i) to investigate sensitivity of a wide range of model outcomes, not only the values of individual output variables; (ii) to examine sensitivity to changes which are not small; (iii) to find efficiently features such as critical or near-redundant parameter combinations. Requirements such as output ranges, credible behaviour or given rank order of scenario outcomes define an *acceptable outcome set*. SA then explores the *feasible set* of parameter values producing acceptable outcomes. This inverts the mapping by the model from parameters to outcomes.

Existing techniques for inverting an output set through a non-linear model work only on small numbers of parameters and outputs, and assume that the output set is bounded by either a box (pairs of bounds on individual variables) or an ellipsoid. Consequently it is proposed to simplify SA by set inversion by two tactics. First, the model is split into simpler sections, *e.g.* with linear dynamics, to allow use of efficient, approximate inversion methods such as ellipsoidal, orthotopic or parallelotopic bounding. Second, attention is confined to features of the feasible set which can answer specific questions, such as largest or smallest diameter, indicating the least and most critical linear parameter combinations. Numerical search from approximate bounds, computed with the help of standard bounding algorithms, is contemplated to find such features.

Even with these tactics, SA by set inversion faces several difficulties:
(i) Approximation error increases as the set is propagated through stages of the model. Existing algorithms process many successive bounded-error output observations one by one, updating the feasible parameter set with the bounds inferred from each by a one-step model inversion. By contrast, SA by set inversion through a non-linear model is likely to handle only a modest number of output bounds, but may have to propagate each through a cascade of model sections. This raises new variations on the problems tackled by established set-inversion algorithms. They produce bounds on model parameters or state from bounds on outputs, whereas SA by set inversion through a number of model sections requires bounds on inputs to all but the last section.
(ii) Almost all existing algorithms produce outer-bound approximations to the feasible set, whereas for SA a conservative estimate of the parameter range is required, *i.e.* inner bounds.
(iii) The standard algorithms assume instantaneous bounds on each output variable or an ellipsoidal instantaneous bound on a vector of outputs. If the flexibility of set-inversion SA is to be exploited, bounds in other metrics have to be permitted.
(iv) Some non-linearities effectively contain switches which can disconnect parts of the model. It is not obvious whether inversion of a bound through such a switch is possible.
(v) A model with stable dynamics has an unstable inverse.

The significance of these difficulties and the factors affecting their resolution are outlined in the paper, with particular reference to how established parameter-bounding algorithms fit into the new scheme.

1. INTRODUCTION

This paper gives the background to a recently started project to explore a new approach to sensitivity assessment (SA) of complex simulation models for natural-resource management. The project partners are The Australian National University, the Universities of Adelaide and Melbourne, the Murray-Darling Basin Commission and the South Australia Department of Water, Land and Biodiversity Conservation. The aims are (i) to investigate sensitivity of a wide range of model outcomes, not confined to values of individual output variables, to variation in parameter values; (ii) to examine non-local sensitivity behaviour, *i.e.* sensitivity to changes which are not small; (iii) to find selected sensitivity features, such as critical or near-redundant parameter combinations, efficiently.

Section 2 reviews SA for models intended to support natural-resource management. The features of such models affecting SA are discussed and the standard approaches to SA, with their limitations, are outlined. An alternative approach, employing bounds on parameters and variables in the model, is motivated and presented in Section 3. Section 4 discusses the scope for using existing tools to implement the approach, the differences between the requirements of the new SA approach and the problems addressed by the existing tools and the resulting difficulties. Fundamental limitations of the approach are also noted.

2. SENSITIVITY ASSESSMENT OF MODELS FOR NATURAL-RESOURCE MANAGEMENT

2.1 Features of NRM Models Affecting Sensitivity Assessment

Models for natural-resource management have several features which make their analysis more difficult: (a) heterogeneity, as they deal with multiple aspects of a situation, *e.g.* hydrological, forest-management, cropping, climatic, economic, ecological, amenity; (b) unavoidable complexity, often simply because the model has both time and location as independent variables and must have a large number of space-time samples for adequate coverage; (c) absence of mathematical properties which simplify analysis: they are typically non-stationary (notably because of year-to-year variation in climate or longer-term climate change, depending on time scale) and sharply non-linear (due, for instance, to changes in water extraction at irrigation-rule thresholds, abrupt hydrological changes due to cropping or farm dams, dependence of flow and erosion mechanisms on rainfall intensity and soil condition, and hard constraints on land use and water availability); (d) incomplete and often unconvincing testing against data, leaving doubts whether the model was fitted to observations *in conditions similar to those pertaining in its intended use*, whether its structure is too elaborate, and whether "validation" against other records, strictly only checking that invalidity is not proven, can establish reliability; and (e) high uncertainty in many of the values of parameters, boundary conditions and inputs supplied to the model, and in structural features such as dynamical order or assumed constancy of parameters.

These features all raise questions about the utility of predictions by the model as guides to the effects of management action. SA is essential if anything better than guesses at the reliability of model responses is to be provided. These same features make SA demanding. Although the need for SA is widely accepted and well established techniques exist (Saltelli *et al*., 2000), SA of models for natural-resource management is rarely fully satisfactory, for reasons discussed below.

2.2 Sensitivity Analysis Through Derivatives

If the relation between the parameters, forcing and/or boundary conditions of interest (henceforth just called parameters) and responses of a model (any specified functions of the model outputs) are continuous and not strongly non-linear, the sensitivities can usefully be defined as the rates of change (derivatives) of the response with respect to the parameters, normalised as appropriate. They can be found by differentiating the model equations with respect to those parameters, then solving the resulting influence equations to find the derivatives. The model will usually include differential equations (DE's), so some influence equations will be DE's, which must be integrated to get the sensitivities as functions of time and perhaps location. Unless the DE's are all linear (and perhaps even then), the integration must probably be numerical, giving results for specific initial conditions, forcing, times and locations, not yielding the insight obtainable from a general analytical solution. The same applies if derivatives are found as finite-difference approximations from many parameter-perturbation runs.

For linear models, SA by finding derivatives has a long history (Tomovic, 1976). Additional assumptions, specifying the probability density functions (pdf's) of the varying parameters, permit uncertainty analysis (Atherton *et al*., 1975). Sensitivity analysis of DE models continues to receive attention, especially from reaction kineticists (Horenko *et al*., 2005).

This approach to SA has fundamental limitations. The first is due to non-linearity. The change in response due to given parameter changes can be found from first derivatives only if the response is near-linear in the parameter; otherwise, the sensitivities vary with the values of the parameters. To use derivatives to find the effects of changes large enough for non-linearity to show, Taylor-series expansion with higher derivatives is required. The number of derivatives may be very large and can only be found by extensive analysis or trial and error, often impracticable. Even if the response is linear in individual parameters, higher derivatives must be found to determine any interaction effects of changing more than one parameter. The second drawback is that little insight is conferred by a mass of derivative values. Further analysis is necessary to find, for instance, what parameter combinations are critical and which might be replaced by simpler combinations.

2.3 Sampling-Based Sensitivity Assessment

Variation of sensitivities with the parameters can be taken into account by random or systematic sampling of the parameters to see how the response varies over their whole realistic range. Systematic sampling schemes such as the Morris method (Morris, 1991) cover all parameter combinations and their entire ranges, and give an indication of the strength of interaction effects, as statistics of the mean and variability of the output changes over a collection of parameter samples. Alternatively, Monte Carlo sampling can be performed, according to distributions specified for the parameters. However, it blurs the distinction between sensitivity assessment and uncertainty assessment. SA aims simply to find how sensitive the responses are to parameter changes and does not need to know anything about the probability properties of the parameters. Uncertainty assessment is usually treated as investigating statistics of the response variations due to parameter variation with given statistics (or, ideally, the relations between the pdf's).

For either deterministic or Monte Carlo sampling, the design problem is to find a scheme to produce the best coverage with an acceptable computing load. There is a risk that significant features of the relations between parameters and outputs are missed because the samples are too sparse. For example, coverage of near-extreme responses is a particular concern. When probability distributions for the parameters can be supplied, stratified sampling allows control of the proportion of samples close to the parameter extremes, but extreme responses may not correspond to extreme parameter values and may still be missed. A similar risk arises with deterministic sampling.

Specialised schemes offer more limited information with greater computing economy. If it is sufficient to apportion the mean-square variation of the response to uncertainties in various parameter combinations, Fourier Analysis Sensitivity Testing (FAST) (Saltelli *et al*., 2000) does so efficiently. Where the response is near-linear in the parameters, principal-component analysis of parameter-sampling results can show which combinations are most and least important.

To avoid imposing too large a computing load, sampling-based SA covers the region of parameter space of interest as thinly as necessary and examines restricted aspects of the output behaviour. A distributional approach to summarising a large body of results is often adopted to avoid the difficulty or impossibility of interpreting the results in detail. The alternative approach outlined below allows a wide range of output behaviour to be nominated as of interest, and does not require or utilise any distributional information. It also offers some prospect of efficient computing by exploiting existing techniques developed in the fields of system identification and state estimation.

3. SENSITIVITY ASSESSMENT BY SET INVERSION

To date, SA methods treat SA as a forward problem, rerunning the model for a range of parameter values and/or boundary conditions. By contrast, the project in progress at ANU and the Universities of Adelaide and Melbourne views SA as the *inverse problem* of translating specified output behaviour back through the model to constrain the parameters. There are three motives for doing so.

First, it fits the questions in SA, which can usually be posed as asking over what parameter range the outputs meet stated requirements. For instance, the ranking order of outputs in a number of scenarios (*e.g.* management policies or climate futures) may be of interest. For preferences to be attached to the outcomes, the order must remain unchanged over a parameter range dictated by prior experience, analysis of model uncertainties or "what if?" considerations. Another example is wishing to know over what parameter range particular outputs, such as salinities at specified places, stay below certain levels. A third instance is asking what relative changes in different parameters cause a given response change.

The second reason for treating SA by model inversion is that it directly exposes model-structure defects. Over-parameterisation shows as a very large range of some parameter combination while still meeting the output requirements, *i.e.* as those parameters being jointly ill defined. Conversely, a very restricted range for a parameter combination indicates that it is critical, and may suggest that the model has too few degrees of freedom.

The third motive is that many techniques exist for inverse problems, translating uncertain output values into uncertain parameter or state values; some may be exploitable for SA. Most parameter-estimation algorithms (Ljung, 1995; Söderström and Stoica, 1989; Norton, 1986) optimise the fit of model outputs to observed output values, but are justified by properties such as statistical consistency, efficiency and asymptotic normality. Those which produce estimates of parameter variability (usually a covariance) translate output variation into parameter variation, so they might in principle be modified for uncertainty assessment.

However, there is an easily interpreted non-probabilistic alternative, apparently relevant to SA treated as turning output requirements, expressed as inequality constraints, into bounds on the parameters. Parameter-bounding identification (Fogel and Huang, 1982; Milanese and Belforte, 1982; Walter, 1990; Norton, 1994, 1995; Milanese *et al*., 1996) finds (approximately in most cases) the *feasible set* of all parameter values giving outputs fitting a sequence of observations to within a given maximum instantaneous error. Parameter-bounding algorithms are well developed for linear dynamical systems (Walter, 2003; Norton, 2003) but less so for non-linear systems (Keesman, 2003; Lahanier *et al*., 1987; Jaulin and Walter,1993; Jaulin *et al.,* 2001). In a closely analogous way, SA can be regarded as finding the feasible set of parameter values corresponding to an *acceptable outcome set* defined by inequality constraints on the output behaviour. These reflect the intended use of the model, as outlined above. SA then looks like a generalisation of parameter bounding, allowing a wider selection of response constraints than bounds on individual output samples.

The idea of finding parameter values making the model response observe specified bounds is the basis of Regional Sensitivity Analysis (RSA) (Spear *et al*., 1994), initially developed in the 1970's. The model is run forwards for a large number of random samples of the parameters, checking the responses against inequality constraints to see if each sample is feasible. RSA then uses the extent and shape of the collection of feasible values to find relatively important and unimportant parameter combinations and hence refine model structure. The method has the big advantage of not requiring linearity. It shares with the proposed set-inversion SA approach great flexibility in specifying what the model outputs must do. Its drawback is a high likelihood of inefficiency. Typically only a small proportion of trial values turn out to be feasible, as the feasible set occupies a small part of the volume of parameter space explored; a much smaller fraction still shows where the boundary of the feasible set lies. Commonly in heavily parameterised environmental models, some parameters are near-redundant, and so the feasible set lies almost in a subspace of parameter space. A further difficulty in predefined sampling SA schemes is the need to know in advance what parameter ranges to explore. As a primary aim of SA is to find out what ranges are significant, this is a Catch 22, to be resolved by trial and error. Both drawbacks are avoided by inversion of the output set.

4. SCOPE FOR EXISTING TOOLS IN SET-INVERSION SA

4.1 Bound Updating

Interest in the variation of outputs of a model (a set of equations) as parameters or boundary conditions vary over specified ranges is common to many fields (Puig *et al*., 2005). Certain generic difficulties in translating parameter variation into output variation or *vice versa* have been recognised. One arises as successive updates of the bounds are carried out, in parameter-bounding identification to impose new parameter bounds inferred from successive output observations, or in SA to propagate bounds through stages of the model. The updates tend to make the feasible set more complicated, so in most cases it has to be approximated by a simpler set. For set inversion in linear dynamical systems, relatively cheap algorithms have been developed to update an ellipsoid (Fogel and Huang, 1982; Pronzato and Walter, 1994; Maksarov and Norton, 1996, 2002) or parallelotope (Chisci *et al*., 1996; Chisci *et al*., 1998) approximating the feasible set of parameters or state variables. Error is incurred at each update of the set and it may well become an unacceptably loose fit to the actual feasible set. This is sometimes called the *wrapping effect*. The effect occurs in both forward and inverse translation of sets through a model.

Fewer updates are likely to be needed for SA by set inversion than for parameter-bounding identification. The latter takes an update to process each output observation, of which there are usually many. In SA by inversion of the acceptable output set, the number of updates at most equals the number of output bounds, provided each update can be performed in a single step back through the model. This is so if the parameter-to-output relation is linear. If the relation is non-linear, updating is not straightforward, as discussed below. Bounds on more than one scalar function of the outputs may sometimes be replaceable by a single approximate (*e.g.* ellipsoidal) joint bound, reducing the number of updates.

The next subsection discusses how output bounds are propagated through time and through a series of model sections, with a view to applying existing parameter- or state-bounding algorithms to update parameter bounds for SA in linear models (model sections taken as near-linear or linearised models valid over a restricted period).

4.2 Updating of Parameter Bounds in Set-Inversion SA for Linear Models

Consider a general linear, time-invariant model expressed in state-space form:

$$\mathbf{x}_k = \mathbf{F}\mathbf{x}_{k-1} + \mathbf{G}\mathbf{u}_{k-1}; \quad \mathbf{y}_k = \mathbf{H}\mathbf{x}_k \tag{1}$$

relating input vector **u** to output **y** *via* state **x** and giving the dynamics of the transition between sample instants k-1 and k. If the model applies over j sample intervals up to time k,

$$\mathbf{y}_k = \mathbf{H}(\mathbf{F}^j\mathbf{x}_{k-j} + \sum_{i=1}^{j}\mathbf{F}^i\mathbf{G}\mathbf{u}_{k-i}) \tag{2}$$

so linear bounds on $\mathbf{y}_k$ imply linear bounds on parameters appearing linearly in **G** or **H** (such as individual elements), but the implied bounds are of degree j in parameters appearing linearly in **F**. Bounds on output behaviour more than one sampling interval later thus impose non-linear bounds on parameters appearing linearly in **F**, and their updating cannot be performed in one step over j sampling intervals if it is to use any of the standard algorithms, which require linearity.

The non-linearity is not avoidable by updating in j steps. Linear bounds on $\mathbf{y}_k$ imply linear bounds on $\mathbf{x}_k$, but thence bilinear bounds on $\mathbf{x}_{k-1}$ and the parameters of **F** jointly, and so on. At each stage the state depends on the parameters in **F** through earlier transitions (1), so the inferred bounds are of degree one higher in those parameters for each step back in time. No such problem occurs for parameters applying at only one instant, *e.g.* input or initial-condition values.

In a sectioned model, bounds may have also to be propagated back through a series of sections. Consider the cascade

$$\left.\begin{aligned}\mathbf{x}_{m,k} &= \mathbf{F}_m\mathbf{x}_{m,k-1} + \mathbf{G}_m\mathbf{u}_{m,k-1}\\ \mathbf{u}_{m+1,k} &\equiv \mathbf{y}_{m,k} = \mathbf{H}_m\mathbf{x}_{m.k}\end{aligned}\right\} m = 1,\ldots,M \tag{3}$$

where m indexes sections and k time. Here the outputs from section m feed section m+1. Bounds on parameters of the transition matrices $\mathbf{F}_1$ to $\mathbf{F}_M$ suffer the complication described above. To bound parameters of $\mathbf{G}_1$ or $\mathbf{H}_1$, bounds on $\mathbf{y}_{m,k}$ must be translated into bounds on $\mathbf{x}_{m,k}$, hence joint bounds on $\mathbf{x}_{m,k-1}$ and $\mathbf{u}_{m,k-1}$, hence bounds on $\mathbf{x}_{m,k-2}$, $\mathbf{u}_{m,k-2}$ and (through $\mathbf{y}_{m-1,k-1}$ and $\mathbf{x}_{m-1,k-1}$) $\mathbf{x}_{m-1,k-2}$ and $\mathbf{u}_{m-1,k-2}$, and so on. Clearly the influence of the parameters in $\mathbf{G}_1$ or $\mathbf{H}_1$ not only travels downstream but also persists through the dynamics. In this linearity is preserved, but the cataloguing of the inferred bounds from bounds on $\mathbf{y}_{m,k}$ to arrive at time-spread bounds on $\mathbf{G}_1$ or $\mathbf{H}_1$ will be a significant burden unless M is small. Furthermore, the standard set-inversion algorithms consider inversion from output to parameters (*e.g.* Fogel and Huang, 1982) or from outputs to state variables (*e.g.* Maksarov and Norton, 1996, 2002), but not outputs to inputs. They must be modified to deal with stage-by-stage set-inversion SA.

If the series of model sections has no dynamics, bound propagation back through the series needs only easily implemented linear transformations.

4.3 Inner-Bounding Approximation of the Feasible Set

Conventional parameter or state bounding seeks not to exclude any feasible values, so it employs outer-bounding approximations. In SA, it is safer to underestimate than to overestimate the parameter range keeping outputs within the prescribed set, so inner-bounding approximation is needed. Inner bounds have seldom been considered (Norton, 1989; Vicino and Milanese, 1991). A potential problem in inner bounding is that loosening of the bounds by cumulative approximation error can lead to the approximated feasible set vanishing. This is less likely in propagating bounds back through a model, where they will usually widen, than in parameter-bounding identification, where the bounds tighten as more observations are processed. Even so, conservative bounds may give a false impression that the parameters are critical, so they will need to be checked by forward model runs.

4.4 Bound Metrics

The acceptable output set may be defined by bounds on a wide variety of aspects of behaviour. For instance, bounds on behaviour over a period of time or a spatial region may be specified, or on how much of the time a condition is met. By contrast, most work on parameter or state bounding assumes instantaneous linear or ellipsoidal bounds on parameter or state vectors. At first sight this discrepancy is serious, but the scope of instantaneous bounds can be extended greatly by augmenting the model with variables which form the desired functions of the outputs. For example, a discrete-interval integrator (summer) can integrate an output variable over a period or region. With a further signum function (switching from 0 to 1 as its input passes a specified value) and a counter, it can register the proportion of the time or space in which a threshold is exceeded.

A signum function switches at its input threshold, as at spilling of a storage. Switches are common in simulation models. The question arises whether a bound can be propagated back through a switch which spends part of the time open. It can. While the switch is closed (the threshold is exceeded), the switch is invisible; while it is open, the bound simply does not apply to the upstream input of the switch. However, in this case there is an implied bound that the upstream variable has not reached the switch threshold. Where bounded downstream variables are affected by other variables as well as the switch output, a bound will have to be propagated back in two parts, taking the switch as closed and open.

4.5 Unstable Inverses

The inverse of a stable model is unstable, so small changes in outputs become large errors in inputs. This is easy to see for a linear model, as the eigenvalues of the inverse are the reciprocals of those of the model, but it is more generally true: if the model is dissipative, its inverse generates energy. In SA, the significant dynamics are from the parameters to the outputs, but this does not alter the essentials. Does instability of the relations between outputs and parameters imply that model inversion is doomed? No: if the proportional effects of changes in parameters are attenuated as they pass through the model, a small change in an affected output corresponds to a large parameter change. This is a valid conclusion.

5. CONCLUSIONS

A new approach has been outlined for sensitivity assessment of simulation models. It translates specified inequality constraints on output behaviour into constraints on model parameters. The approach offers flexibility in stating what is important in the outputs. By determining the joint ranges of the parameters, it has potential for revealing critical or near-redundant parameter combinations. It does not rely on any probabilistic knowledge and does not assume small variations.

Existing parameter-bounding techniques may be helpful in turning output bounds into parameter bounds, but as discussed above, several features of SA by model inversion make their exploitation far from simple. In practice, it is not necessary or desirable to find a full description of the set of parameter values consistent with the output constraints. Judicious selection of features to identify, together with complementary use of numerical search (not discussed in detail here), may be crucial to success of the approach.

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