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A review of foundational methods for checking the structural identifiability of models: Results for rainfall-runoff

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SUMMARY

Checking for model identifiability has several advantages as outlined in the paper. We illustrate the use of several screening methods for assessing structural identifiability that should serve as a valuable precursor to model redesign and more sophisticated uncertainty analyses. These are: global evolutionary optimisation algorithms (EAs) that are being used increasingly to estimate parameters of models because of their flexibility; one and two-dimensional discrete model response plots with the latter showing trajectories of convergence/non-convergence; quadratic response surface approximations; and sensitivity analysis of combinations of parameters using Polynomial Chaos Expansion model emulation. Each method has a role to play in understanding the nature of non-identifiability. We illustrate the utility and complementary value of these methods for conceptual rainfall-runoff processes with real and 'exact' daily flow data, hydrological models of increasing complexity, and different objective functions. We conclude that errors in data are not primarily the cause of the parameter identification problem and objective function selection gives only a partial solution. Model structure reveals itself to be a major problem for the two more complex models examined, as characterised by the dotty/1D, 2D projection and eigen plots. The Polynomial Chaos Expansion method helps reveal which interactions between parameters could affect the model identifiability. Structural non-identifiability is seen to pervade even at modest levels of model complexity.

1. Introduction

The hydrological modelling community has in recent years shown a strong interest in the issue of uncertainty in model identification and parameter estimation. From this literature, Wagener and Gupta (2005) differentiate three philosophical approaches to parameter uniqueness: *equifinality*, by which the modeller should expect to find multiple acceptable models; *parsimony*, which aims for models to be as simple as possible, but no simpler; and *power*, which advocates the need to improve model identification techniques to make better use of available information.

A key concept related to parameter uniqueness is structural identifiability. Structural non-identifiability (Koopmans and Reiersol, 1950; Bellman and Åström, 1970; Rothenberg, 1971) occurs if a model is found to have non-unique parameters due to model structure, input and outputs, even when 'exact' model inputs and output data are used in conjunction with a given objective function and constraints.

Understanding of structural identifiability is essential to all of Wagener and Gupta's philosophical approaches. In terms of the framework for assessing model structural adequacy proposed by Gupta et al. (2012), structural identifiability is notably influenced by equation structure, which determines the parameters selected and how they are theoretically related, and computational structure, which determines the computational interactions between parameters. These are foundations that need to be strengthened regardless of how the broader concept of parameter uniqueness

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is approached in the long run. An equifinality approach needs to know if the multiple models are in fact identical because of mathematical rather than catchment properties, and might even all be unacceptable (Beven, 1993, 2006). A large parameter space of acceptable solutions may be attributable to lack of identifiability of parameters (Beck, 1987). A parsimonious approach needs to use identifiability analysis techniques to judge whether a model is too complex. Structures of even moderately complex models can be non-identifiable, as we will show. Finally, improving power of a model requires diagnosis and learning about the causes of existing problems, which Gupta and Nearing (2014) argue should be a research priority.

As a minimum it seems that the nature of the identifiability problem for a given model and its context warrants investigation for one or more reasons such as:

1. to understand the model better especially its limitations, parameter sensitivities and interactions;
2. to aid in redesign of a model that is more identifiable and perhaps simpler;
3. to help seek parameter values that have less ambiguous process or characteristic responses so that the model is useful for providing interpretable insight into the behaviours it captures;
4. to reduce the chances of a model predicting inadequately on independent datasets; and
5. to examine the role of objective functions and constraints in uncertain parameter estimation.

Methods to screen for identifiability problems are readily available, but not commonly used as partially demonstrated by the literature review of Shin et al. (2013) on the seldom reported use of sensitivity analysis of hydrological models. The authors feel that the hydrological community stands to benefit greatly from wider awareness of identifiability issues and the complementary nature of some of the tools available. Identifiability analysis classically gives an answer in the form of “yes” or “no” as to whether unique parameter estimates can be identified (e.g. Norton, 1980; Walter and Lecourtier, 1981). But it can be undertaken to assess the numerical values of the unknown parameters and the associated extent of the identification accuracy (e.g. Wagener et al., 1999, 2001a, 2001b; Wagener and Kollat, 2007; Mejía and Moglen, 2010; Zégre et al., 2010; Muñoz et al., in press). For largely hydrological applications there have been several identifiability analysis studies including: quantifying, removing or reducing correlation between model parameters (Gupta and Sorooshian, 1983; Dochain et al., 1995); comparison of collinearities and magnitudes of relative sensitivities to calculate a rank that indicates which of the parameters can be identified (Brun et al., 2001); quantification of data worth through its effect on parameter identifiability (Brunner et al., 2012); time-varying sensitivity analysis for hydrological models with different complexity (Herman et al., 2013). But there appears to be scope for assessing the function of different methods that indicate or characterise model non-identifiability, and the roles that each method can play.

At its most obvious, the problem of identifiability is encountered by modellers when optimisation-based parameter estimation yields different solutions depending on the initial values used. As will be shown, this lack of convergence can occur even when the most sophisticated global optimisation algorithms are applied. It may be due to (i) errors in data and model, (ii) objective function selection, and (iii) poor model structure such as due to over-parameterisation and/or model bias (Sorooshian et al., 1993; Andréassian et al., 2012). The difficulties in convergence can result from the generation of multiple parameter sets that have multiple equifinal solutions (i.e. a unique solution is not identifiable). The above convergence difficulties, even when robust Evolutionary Algorithms (EAs) are used for the calibration, have been indicated in the water resources literature. The studies of Gupta and Sorooshian (1985), Sorooshian et al. (1993) and Valent et al. (2012) have indicated such parameter variation, as have van Werkhoven et al. (2009) who generated Pareto fronts using multiple starting values of the EA and different objective functions.

This paper investigates the structural identifiability problem for conceptual rainfall-runoff models, and implies lessons for other types of models. While the paper does focus on the role of non-uniqueness by using ‘exact’ models and data, it also indicates that the role of data errors is subsidiary for the models and data sets investigated. In other words there is a basic structural problem of non-uniqueness for some commonly used models and the amount of identifiability caused by errors for these models does not seem important. Nor does the use of more complex objective functions selected seem helpful. Of course this is not to say that other objective functions, and indeed constraints, could not be found that assist in reducing the non-uniqueness. Other climatic forcing data might also inform the optimisation more, but we did apply daily data from five catchments, each of 40 years duration and covering quite a wide range of variability in the nature of that forcing.

In the following we demonstrate four foundational techniques focussed on understanding the context and causes of convergence and identifiability problems that:

- Check whether multiple parameter estimations with different initial values obtain a unique solution.
- Visualise the EA solutions in greater context using one and two-dimensional parameter response surface plots.
- Model the response surface with a second-order polynomial regression to quantify pair-wise parameter interactions and identifiability, a technique known as the Response Surface Methodology (RSM).
- Use global sensitivity analysis to identify the effect of interactions between multiple parameters. Several methods can be used, including using Sobol sequences and modelling the response surface with Polynomial Chaos Expansion (PCE) methods.

Section 2 presents each of these methods. In Section 3, we present or refer to a brief description of the catchments, the rainfall-runoff models, the input data and the objective functions. In Section 4 we present our results. The discussion and conclusions are given in Section 5.

2. Identifiability screening methods

2.1. Evolutionary Algorithms (EAs)

An identifiability problem generally exists if multiple global parameter estimations fail to obtain the same unique solution. This paper repeats parameter estimation with 10 sets of randomly selected initial parameter values, using each of five well-known evolutionary algorithms.

The EAs used in the study are: the Shuffled Complex Evolution (SCE) algorithm, the Differential Evolution (DE) algorithm, the DiffeRential Evolution Adaptive Metropolis (DREAM) algorithm, the Covariance Matrix Adaptation Evolution Strategy (CMAES) algorithm and Non-dominated Sorting Genetic Algorithm II (NSGA-II). The five EAs were selected because they have been widely used in recent hydrological modelling studies. Note that gradient descent local optimisation algorithms (e.g. Nelder-Mead, Quasi-Newton, Gauss–Marquardt–Levenberg, etc.) which are, by far, the fastest methods to find optimal parameter values were not consid-