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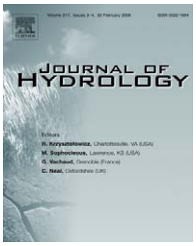

Efficient accommodation of local minima in watershed model calibration

Brian E. Skahill [a,*], John Doherty [b]

[a] *Coastal and Hydraulics Laboratory, U.S. Army Engineer Research and Development Center, Hydrologic Systems Branch, Waterways Experiment Station, 3909 Halls Ferry Road, Vicksburg, MS 39180, USA*
[b] *Department of Civil Engineering, University of Queensland, St. Lucia, Australia 4068, Watermark Numerical Computing, Brisbane, Australia*

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Summary The Gauss–Marquardt–Levenberg (GML) method of computer-based parameter estimation, in common with other gradient-based approaches, suffers from the drawback that it may become trapped in local objective function minima, and thus report ''optimized'' parameter values that are not, in fact, optimized at all. This can seriously degrade its utility in the calibration of watershed models where local optima abound. Nevertheless, the method also has advantages, chief among these being its model-run efficiency, and its ability to report useful information on parameter sensitivities and covariances as a by-product of its use. It is also easily adapted to maintain this efficiency in the face of potential numerical problems (that adversely affect all parameter estimation methodologies) caused by parameter insensitivity and/or parameter correlation.

The present paper presents two algorithmic enhancements to the GML method that retain its strengths, but which overcome its weaknesses in the face of local optima. Using the first of these methods an ''intelligent search'' for better parameter sets is conducted in parameter subspaces of decreasing dimensionality when progress of the parameter estimation process is slowed either by numerical instability incurred through problem ill-posedness, or when a local objective function minimum is encountered. The second methodology minimizes the chance of successive GML parameter estimation runs finding the same objective function minimum by starting successive runs at points that are maximally removed from previous parameter trajectories. As well as enhancing the ability of a GML-based method to find the global objective function minimum, the latter technique can also be used to find the locations of many non-global optima (should they exist) in parameter space. This can provide a useful means of inquiring into the well-posedness of a parameter estimation problem, and for detecting the presence of bimodal parameter and predictive probability distributions.

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[*] Corresponding author. Tel.: +1 601 634 3441; fax: +1 601 634 4208.
E-mail address: brian.e.skahill@erdc.usace.army.mil (B.E. Skahill).

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The new methodologies are demonstrated by calibrating a Hydrological Simulation Program-FORTRAN (HSPF) model against a time series of daily flows. Comparison with the SCE-UA method in this calibration context demonstrates a high level of comparative model run efficiency for the new method.

Introduction

Computer-based calibration of surface water quantity and quality models generally involves minimization of an ''objective function'' – a measure of model-to-measurement misfit. In simple cases this is comprised of differences between measured and modeled flows at, for example, daily, hourly or even smaller intervals. In many cases, observed and modeled flows are transformed (for example through a Box-Cox transformation) before fitting, and/or residuals are fitted to an ARMA model prior to formulation of an objective function, in order to reduce heteroscedascity and temporal correlation (Box and Tiao, 1973; Box and Jenkins, 1976; Kuczera, 1983; Bates and Campbell, 2001). In more complex cases a multi-criterion objective function is constructed in which different measurement types, or the same measurement type processed in different ways, comprise separate components of a composite global objective function (Madsen, 2000; Boyle et al., 2000; Doherty and Johnston, 2003).

A unique solution to the inverse problem of model calibration can only be guaranteed if the information content of a calibration dataset is sufficient to allow values to be assigned to all parameters for which estimation is sought through the calibration process. Often this is ensured by adherence to the so-called ''principle of parsimony'' in design of the inverse problem, whereby the number of parameters for which estimated values are sought is kept to a minimum while at the same time retaining enough parameters to allow a satisfactory fit between model outputs and field data to be achieved (Hill, 1998). It is often recommended that, prior to model calibration, a sensitivity analysis be conducted to identify those parameters that are estimable and those that are not; the latter are then fixed at realistic values while the ''identifiable'' parameters are estimated. Unfortunately however, especially where models are highly nonlinear, it is the parameter estimation process itself that is the final arbiter of parameter identifiability, for it is not always possible to select an appropriate subset of parameters for estimation ahead of actually undertaking the parameter estimation process. If too few parameters are selected for estimation, the calibration objective function will not be lowered to the extent that it possibly could be if other parameters were involved in the inversion process. However, in some cases the involvement of these extra parameters may lead to nonuniqueness in their estimation and, depending on the parameter estimation package employed, possibly poor performance of that package due to consequential numerical instability. Furthermore, even if the parameter estimation process is successful in minimizing the objective function under these circumstances, the final parameter set will lie within a long valley that defines the loci of objective function minima in parameter space. Should such a valley (rather than a bowl containing a unique minimum) exist, the parameter estimation package should notify the user of this, and of the fact that parameter estimates forthcoming from the calibration process are nonunique.

Whether or not an inverse problem is poorly posed, and whether or not the objective function minimum is elongate or round, it is rarely possible to avoid the fact that when calibrating watershed models the objective function will often contain local minima in addition to its global minimum; see Duan et al. (1992) for a full discussion of this topic. This presents challenges to the design of automatic calibration software, for a modeler who uses such software has the right to expect that estimated parameter sets result in the best possible fit between model outputs and field measurements (with due account taken of parameter believability). Ideally, however, a modeler would also like to receive some information from a calibration package on the locations of non-global minima, especially if these minima are little different in magnitude from the global minimum, but are widely separate from it in parameter space. Indeed, information on the structure of the objective function surface can be of great assistance in allowing a modeler to qualitatively appraise the linearity and utility of his/her model, the uncertainty of parameters estimated though the parameter estimation process, and the information content of the dataset that is currently available for its calibration (Sorooshian and Arfi, 1982; Kuczera, 1990).

A further consideration in assessing the performance of a parameter estimation package is that of run time. Parameter estimation software, no matter what its algorithmic basis, must run the model whose task it is to calibrate many times in the course of minimizing the objective function that is used to characterize model-to-measurement misfit. Where model run times are high, model run efficiency of the calibration process becomes of paramount concern. It is inevitable that the challenges posed by parameter nonuniqueness and local objective function minima will lead to the necessity to carry out more model runs than that required for solution of an inverse problem characterized by a convex objective function surface with a single minimum. However, if the cost of meeting these challenges is too high, a parameter estimation package may simply be unusable in many modeling contexts, despite what may be a high degree of numerical robustness.

Choice of parameter estimation package

Much has been written concerning the suitability of various parameter estimation strategies for calibration of watershed models; see for example Thyer et al. (1999),