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Parameter and modeling uncertainty simulated by GLUE and a formal Bayesian method for a conceptual hydrological model

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SUMMARY

Quantification of uncertainty of hydrological models has attracted much attention in hydrologic research in recent years. Many methods for quantification of uncertainty have been reported in the literature, of which GLUE and formal Bayesian method are the two most popular methods. There have been many discussions in the literature concerning differences between these two methods in theory (mathematics) and results, and this paper focuses on the computational efficiency and differences in their results, but not on philosophies and mathematical rigor that both methods rely on. By assessing parameter and modeling uncertainty of a simple conceptual water balance model (WASMOD) with the use of GLUE and formal Bayesian method, the paper evaluates differences in the results of the two methods and discusses the reasons for these differences. The main findings of the study are that: (1) the parameter posterior distributions generated by the Bayesian method are slightly less scattered than those by the GLUE method; (2) using a higher threshold value (>0.8) GLUE results in very similar estimates of parameter and model uncertainty as does the Bayesian method; and (3) GLUE is sensitive to the threshold value used to select behavioral parameter sets and lower threshold values resulting in a wider uncertainty interval of the posterior distribution of parameters, and a wider confidence interval of model uncertainty. More study is needed to generalize the findings of the present study.

Introduction

Conceptual hydrological models are popular tools for simulating the land phase of the hydrological cycle. They are frequently used for water balance analysis, extending and infilling streamflow records, flow forecasting, reservoir operation, water supply, and watershed management. One distinguishing characteristic of a conceptual model is that one or more of its parameters requires calibration using physically observable catchment responses (Kuczera and Parent, 1998). When parameter calibration is employed, it is easy to show that multiple calibration periods yield multiple optimum parameter sets, and even in a single period, different sets of optimum parameter values may yield similar model performances; this is termed as "equifinality" in the literature. On the other hand, for the same input and output data, different models, with similar calibration results, may produce largely different predictions, as observed by Jiang et al. (2007) in a comparison of hydrological impacts of climate change simulated by six hydrological models. Since a conceptual model can be viewed as an empirical combination of mathematical operators describing the main features of an idealized hydrologic cycle, one cannot rely on a uniquely determined model parameter set or model prediction (Kuczera and Parent, 1998). Consequently, attention should be paid to the uncertainties in hydrological modeling.

Generally speaking, there are three principal sources contributing to modeling uncertainty: errors associated with input data and data for calibration, imperfection in model structure, and uncertainty in model parameters (e.g., Refsgaard and Storm, 1996). Xu et al. (2006) demonstrated that the quality of precipitation data influences both simulation errors and calibrated model parameters. Engeland et al. (2005) showed that the effect of the model structural uncertainty on the total simulation uncertainty of a conceptual water balance model was larger than parameter uncertainty. Marshall et al. (2007) stated that the uncertainty in model structure requires developing alternatives, where outputs from multiple models are pooled together in order to generate an ensemble of hydrographs that are able to represent uncertainty. Kavetski et al. (2002), and Chowdhury and Sharma (2007) investigated input data uncertainty by artificially adding noise to input

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data and then formulating an empirical relationship between this noise and parameter error. Many other examples of the methods dealing with model and data uncertainty are available in the hydrological literature (e.g., Georgakakos et al., 2004; Carpenter and Georgakakos, 2004; Kavetski et al., 2006a,b).

A variety of methods have been developed to deal with parameter uncertainty and modeling uncertainty, i.e., to provide posterior distributions for parameters and runoff, which are of greater interest. Among these methods, the generalized likelihood uncertainty estimation (GLUE) method, developed by Beven and Binley (1992), and the formal Bayesian method using Metropolis–Hastings (MH) algorithm, a Markov Chain Monte Carlo (MCMC) methodology, are extensively used (Freer et al., 1996; Beven and Freer, 2001; Kuczera and Parent, 1998; Bates and Campbell, 2001). According to Beven et al. (2000), GLUE "represents an extension of Bayesian or fuzzy averaging procedures to less formal likelihood or fuzzy measures." The concept of "the less formal likelihood", which represents the main element of differentiation with the Bayesian inference, is a remarkable aspect of the GLUE methodology. The flexible definition of the likelihood function allows for no strong assumptions on the error model. Doubtless, when the assumptions are fulfilled, the formal Bayesian method is the most convenient to use, since "the formal Bayesian approach has its roots within classical statistical theory and applies formal mathematics and MCMC simulation to infer parameter and prediction distributions" (Vrugt et al., 2008). At the same time, variants of these methods have also been developed. These include utilizing a new procedure to partially correct the prediction limit of a hydrological model in GLUE (Xiong and O'Connor, 2008), introducing adaptation into the MCMC method (Kuczera and Parent, 1998; Gilks et al., 1998; Yang et al., 2007, 2008), merging one of MCMC sampler with the SCE-UA global optimization algorithm (Vrugt et al., 2003), and revising GLUE based on the MCMC sampling (Blasone et al., 2008a,b), amongst others.

Compared to other methods, GLUE is easy to implement, requiring no modifications to existing source codes of simulation models. Therefore, many users are attracted by GLUE. On the other hand, controversy over GLUE has recently started to increase "for not being formally Bayesian, requiring subjective decisions on the likelihood function and cutoff threshold separating behavioral from non-behavioral models, and for not implementing a statistically consistent error model" (Blasone et al., 2008b). In the same work, Blasone et al. (2008b) pointed out that "... the GLUE derived parameter distribution and uncertainty bounds are entirely subjective and have no clear statistical meaning." Stedinger et al. (2008) argued that although an absolutely correct likelihood function may be difficult to construct, it should not be an excuse to use any function and calls for a likelihood measure that will yield probabilities with any statistical validity. Liu et al. (2005) and Todini (2008) showed that a formal likelihood measure can be derived by first converting a real data set into a normal space.

Another drawback of GLUE is that it is computationally inefficient and can even lead to misleading results, unless a large sample is drawn (Blasone et al., 2008a). Mantovan and Todini (2006) showed the incoherence of GLUE with Bayesian inference using an experiment, where synthetic input and output and a correct formal likelihood function were applied, and they referred it to as pseudo-Bayes. They proved that the "less formal likelihoods" failed to guarantee the requirements of Bayesian inference process that adding more data did not necessarily add information to the conditioning process, and the equivalence of experimental value irrespective of the order. Subsequently, Beven et al. (2007) responded that GLUE was not developed to deal with cases for which every observation added information to the conditioning process. It was developed to deal with real calibration problems in which both inputs and model structural errors played an important role. They further showed that if a correct formal likelihood was used as a prior in GLUE, the results obtained would be identical with the formal Bayes. Stedinger et al. (2008) showed that using a correct likelihood function GLUE can lead to meaningful uncertainty and prediction intervals. Blasone et al. (2008b) also stated that the computational efficiency of GLUE is improved by sampling the prior parameter space using an adaptive MCMC scheme.

It can be noted here that in many cases it is not easy to compare the original GLUE method and the formal Bayesian method directly. First, the formal Bayesian approaches attempt to disentangle the effect of input, output, parameter and model structural error which, on one hand, are important to improve our hydrologic theory of how water flows through watersheds; on the other hand these attempts make statistical inference difficult (Vrugt et al., 2008). GLUE does not attempt to separate these effects on the total uncertainty which, on one hand, makes it easy to use and understand, but on the other hand it is impossible to pinpoint what elements of the model constitute most uncertainty. Second, in practice the formal Bayesian method is often used to calculate the uncertainty interval of one-step ahead forecasting with a formal or exact likelihood function that is assumed or transformed from a more general and unknown form, while the GLUE method is often used to calculate the uncertainty interval of streamflow simulation with a statistically informal likelihood function. In this study, both methods are applied on the same grounds, i.e., our focus is on the computational efficiency and differences in the results of parameter and model uncertainty calculated by the two methods, and not on the different philosophies and mathematical rigor that both methods rely on. Additional analyses are performed to test how sensitive the GLUE results are to the threshold values of retained solutions.

The specific objectives of this paper are: (1) to assess parameter uncertainty of a conceptual hydrological water balance model WASMOD (Xu, 2002) using GLUE and Bayesian method, and (2) to examine the differences in the results of these two methods and discuss the reasons for the differences.

The organization of this paper is as follows. After this brief introduction, two methods are presented, followed by a discussion of the WASMOD model, study area and data used. Then, parameter and modeling uncertainty of the two methods are compared and discussed, and the results and conclusions are presented.

Methods

Formal Bayesian approach

Consider a random variable Y whose value is denoted by y and a parameter vector θ. $P(\theta)$ is a prior distribution of θ based on historical data or expert knowledge, and $L(Y/\theta)$ is the likelihood function based on data collected by observations. The Bayesian theorem provides a formal mechanism for deriving the posterior distribution, $P(\theta/Y)$, of θ based on the prior distribution and likelihood distribution as:

$$P(\theta/Y) = \frac{L(Y/\theta)P(\theta)}{\int L(Y/\theta)P(\theta)d\theta} \propto L(Y/\theta)P(\theta) \quad (1)$$

Based on the investigation by Xu (2001) on the statistical properties of the simulation error for the WASMOD model, a square-root transformation is applied:

$$\sqrt{Q_{obs,t}} = \sqrt{Q_{sim,t}} + \varepsilon_t \quad (2)$$

where $Q_{obs,t}$ is the observed streamflow at time t, $Q_{sim,t}$ is the simulated streamflow at time t, and ε_t is the residual term. It is assumed that this residual term is mutually independent and approximately