Journal of Hydrology (2007) **332**, 303–315

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

Quantifying hydrological modeling errors through a mixture of normal distributions

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Received 28 February 2005; received in revised form 16 May 2006; accepted 13 July 2006

KEYWORDS
Gaussian mixtures;
Modeling error;
Parameter uncertainty;
Bayesian inference;
Rainfall-runoff models;
Metropolis algorithm

Summary Bayesian inference of posterior parameter distributions has become widely used in hydrological modeling to estimate the associated modeling uncertainty. The classical underlying statistical model assumes a Gaussian modeling error with zero mean and a given variance. For hydrological modeling residuals, this assumption however rarely holds; the present paper proposes the use of a mixture of normal distributions as a simple solution to overcome this problem in parameter inference studies. The hydrological and the statistical model parameters are inferred using a Markov chain Monte Carlo method known as the Metropolis–Hastings algorithm. The proposed methodology is illustrated for a rainfall-runoff model applied to a highly glacierized alpine catchment. The associated total modeling error is modeled using a mixture of two normal distributions, the mixture components referring respectively to the low and the high flow discharge regime. The obtained results show that the use of a finite mixture model constitutes a promising solution to model hydrological modeling errors in parameter inference studies and could give additional insights into the model behavior.

Introduction

The quantification of hydrological modeling uncertainties is currently one of the key issues of hydrological research. Especially in the area of conceptual modeling, the uncertainty inherent to any types of prediction is receiving increasing interest. Conceptual models represent a highly simplified description of the natural phenomena underlying a hydrological response. Some of their model parameters can therefore not be measured directly but have to be calibrated using observed data of the simulated catchment response. In the past, the determination of the best or the most probable parameter set has been subjected to intense research (e.g., Duan et al., 1992) whereas current research concentrates on the estimation of the posterior parameter distribution (e. g., Kuczera and Parent, 1998; Vrugt et al.,

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0022-1694/$ - see front matter
doi:10.1016/j.jhydrol.2006.07.005

2003). Monte Carlo methods have become widely used for the Bayesian inference of posterior parameter distributions, the most known in the area of hydrological modeling being the so-called GLUE method (Generalized Likelihood Uncertainty Estimation) (Beven and Binley, 1992) — an importance sampling technique — and different types of Markov Chain Monte Carlo (MCMC) sampling techniques, the most frequently used in hydrological modeling being the so-called Metropolis algorithm (Metropolis et al., 1953).

The Bayesian inference of posterior parameter distributions requires the definition of an appropriate statistical model for the model error distribution to formulate the corresponding likelihood function. In conceptual hydrological modeling, the classical normality assumption is generally not respected, as the modeling residuals are typically not homoscedastic: On one hand, the data that serves to drive and calibrate the model is affected by non-stationary and heteroscedastic errors (e.g., Sorooshian and Dracup, 1980; Vrugt et al., 2005); on the other hand, the errors due to the imperfection of the hydrological model depend on the active components of the model that in turn depend on the input, the system state and the dominating processes at a given time step (e.g., Kavetski et al., 2003; Krzysztofowicz and Herr, 2001).

The potentially non-Gaussian nature of modeling residuals and especially their heteroscedasticity is frequently mentioned in model calibration studies but comparatively seldom explicitly assessed (see, e.g., Bates and Campbell, 2001; Xu, 2001). The assumption of zero expectation is tested in most studies and it is generally well respected by the residuals of calibrated hydrological models; the assumptions of independent and homoscedastic residuals is however frequently violated (see, e.g., Bates and Campbell, 2001; Xu, 2001, and our case study results). The first problem is generally tackled through the introduction of an autocorrelation term in the error model (e.g., Sorooshian and Dracup, 1980).

A popular approach to reduce the heteroscedasticity of the residuals of hydrological models is data transformation (see, e.g., Bates and Campbell, 2001; Thyer et al., 2002; Vrugt et al., 2003). Krzysztofowicz and Herr (2001) apply a normal quantile transform and in addition, condition in their meta-Gaussian model the hydrologic uncertainty on the occurrence or non-occurrence of precipitation. The application of data transformations to make residuals homoscedastic is interesting from a statistical point of view (see, e.g., Box and Cox, 1964), simple to implement and can give good results in hydrological modeling (see, e.g., Bates and Campbell, 2001; Sorooshian and Dracup, 1980; Thiemann et al., 2001). We would however like to point out here that in the context of parameter inference and model uncertainty estimation, the use of transformed data can be questionable and a problem can arise: If we estimate the model parameters in a transformed output variable space assuming that in the transformed space the modeling error has zero mean, the modeling error will not necessarily have a zero mean in the retransformed variable space.

While this result is obvious from a statistical viewpoint and sometimes mentioned in the context of hydrological modeling (see, e.g., Koch and Smillie, 1986; Lane, 1975) we could not find any study that discusses the implications of this problem for hydrologic parameter calibration studies: If the retransformed output variable is used as an input into a further model, part of the input into this model has no hydrological origin but is induced by the modeling error assumption in the transformed data space used for parameter inference. If we model for example discharge for a water management model, this means that part of the water input into the management model is not the result of precipitation — runoff transformation but stems from not explicitly assessed sources (the modeling error). In applications where the estimation of the posterior distribution of the hydrological response is the endpoint of the study, this fact can be neglected and is probably therefore rarely mentioned.

A detailed discussion of the implications of data transformation for hydrological model calibration studies is beyond the context of the present paper. But the highlighted potential pitfall led us to the development of a model error that explicitly excludes data transformation to address the correlation and the heteroscedasticity of the residuals. The error model presented here uses a simple parametric method, a so-called finite mixture distribution that approaches highly complex distributions through a weighted sum of standard distributions such as the normal distribution (see the work of Bardsley, 2003 or Krzysztofowicz and Herr, 2001 and Maranzano and Krzysztofowicz, 2004 for an application in hydrological modeling).

In our application to a precipitation — runoff model, we use a mixture of normal distributions and fix the number of mixture components to two, corresponding respectively to the high flow and the low flow period. This empirical choice is based on a priori information (see case study section) about the sources and behavior of the modeling errors. The parameters of the mixture distribution (and the two normal distributions composing it) are estimated along with the hydrological model parameters through a Metropolis—Hastings algorithm (Hastings, 1970). The properties of the so inferred error distributions — namely the properties of the two normal distributions and the differences between them — can give valuable insights into the model behavior and into its ability to simulate the runoff processes during the two flow periods (see discussion section).

We first present the general formulation of the finite mixture error model, followed by a short overview of the used Metropolis—Hastings algorithm and a short discussion of some relevant implementation aspects. The statistical model and the inference of its parameters are illustrated for a case study in the Swiss Alps. The obtained results show that the use of a finite mixture model constitutes a promising solution to model errors and to estimate the total modeling uncertainty in hydrological model calibration studies.

Finite mixture error model

In parameter inference studies, the catchment response simulated through a hydrological model is generally represented as a non-linear regression of the following form (e.g., Sorooshian and Dracup, 1980; Thiemann et al., 2001):

$$q_t = h(\mathbf{x}_t, \boldsymbol{\beta}) + \delta_t \tag{1}$$

where q_t is the observed hydrological response on time step t ($t = 1, \ldots, n$), $h(\mathbf{x}_t, \boldsymbol{\beta})$ is the hydrological transfer function mapping the inputs $\mathbf{x}_t$ (containing input variables such as