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Improvement and comparison of likelihood functions for model calibration and parameter uncertainty analysis within a Markov chain Monte Carlo scheme

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SUMMARY

In this study, the likelihood functions for uncertainty analysis of hydrological models are compared and improved through the following steps: (1) the equivalent relationship between the Nash–Sutcliffe Efficiency coefficient (*NSE*) and the likelihood function with Gaussian independent and identically distributed residuals is proved; (2) a new estimation method of the Box–Cox transformation (BC) parameter is developed to improve the effective elimination of the heteroscedasticity of model residuals; and (3) three likelihood functions—*NSE*, Generalized Error Distribution with BC (BC-GED) and Skew Generalized Error Distribution with BC (BC-SGED)—are applied for SWAT-WB-VSA (Soil and Water Assessment Tool – Water Balance – Variable Source Area) model calibration in the Baocun watershed, Eastern China. Performances of calibrated models are compared using the observed river discharges and groundwater levels. The result shows that the minimum variance constraint can effectively estimate the BC parameter. The form of the likelihood function significantly impacts on the calibrated parameters and the simulated results of high and low flow components. SWAT-WB-VSA with the *NSE* approach simulates flood well, but baseflow badly owing to the assumption of Gaussian error distribution, where the probability of the large error is low, but the small error around zero approximates equiprobability. By contrast, SWAT-WB-VSA with the BC-GED or BC-SGED approach mimics baseflow well, which is proved in the groundwater level simulation. The assumption of skewness of the error distribution may be unnecessary, because all the results of the BC-SGED approach are nearly the same as those of the BC-GED approach.

1. Introduction

Hydrologists have developed many models based on different theories and concepts, such as SWAT (Neitsch et al., 2005) based on the principle of the hydrologic response unit (HRU), TOPMODEL (Beven and Kirkby, 1979) based on the topographic wetness index (TWI), TOPKAPI (Liu and Todini, 2002) based on the nonlinear reservoir theories, and HBV model (Wrede et al., 2013; Li et al., 2014) based on a modification of the bucket theory in that it assumes a statistical distribution of storage capacities in a basin. However, because of the hydrologic complexity and especially the hydrologic heterogeneity, these models cannot describe the natural hydrologic processes entirely correctly, and their parameters can be interpreted only to the "effective parameters" which represent the integrated behavior at the model element scale. Because it is difficult to determine the "effective parameters" directly from field measurement, the model parameters should be determined through calibration against the historical record data (Laloy et al., 2010). Owing to the lack of sufficient observation data and the inter-dependence of model parameters, equifinality of parameter sets must be expected instead of a single 'optimal' parameter set in calibration against field data (Beven, 2001; Beven and Freer, 2001).

Additionally, errors in input data, model structure and measured outcomes are all lumped into a single additive residual term, and then passed to the model parameters when calibrating the hydrological model (Yang et al., 2007a,b; McMillan and Clark, 2009; Schoups and Vrugt, 2010). The parameter equifinality and errors, individually or combined, result in parameter uncertainty. So, the calibration of model parameters is being developed to include estimation of the probability distribution of parameters

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that represents the knowledge about parameter values (Yang et al., 2007b), and the Bayesian approach (usually using Markov chain Monte Carlo scheme (MCMC)) is popularly proposed (Jin et al., 2010; Li and Xu, 2014). The Bayesian approach (or MCMC) tries to separate the observations (e.g. river discharges) into two parts: a deterministic component and a random component describing residuals (Schoups and Vrugt, 2010). The deterministic component is determined by the hydrologic model. The joint probability of the random component, i.e. residuals/errors between observations and simulations generated by hydrologic model with a particular parameter set, is estimated by a likelihood function. By augmenting the likelihood function with prior knowledge of model parameters, the posterior distribution of model parameters is estimated.

There are many successful applications for calibration and uncertainty analysis of model parameters using the Bayesian approach with the MCMC scheme. For example, McMillan and Clark (2009) used a modified *NSE* (Nash–Sutcliffe Efficiency coefficient (Nash and Sutcliffe, 1970)) as an informal likelihood function to calibrate model parameters. However, the modified *NSE* failed to reveal the relationship between the *NSE* and the likelihood function with statistical assumptions. Stedinger et al. (2008) indicated that the standard least squares (SLS), equivalent to maximizing *NSE*, is a kind of formal likelihood function under the assumption that the errors follow Gaussian distribution with zero mean and a constant variance. This theoretical derivation, however, is non-strict because of fixing the standard deviation of residuals/errors.

In recent years, some doubts have been expressed about the formal Bayesian approach. The two main reasons are summarized as follows (Beven et al., 2012; Clark et al., 2012): First, the formal Bayesian inference mistakenly treated all residuals as random errors; second, there is no generalized likelihood function that could be appropriate for all model structures. Beven et al. (2012) indicated that the model residuals include epistemic errors (such as model structure and input errors) as well. The epistemic errors result in the correlative and heteroscedastic characteristics of model residuals. In order to account for the errors' correlation and heteroscedasticity, many researchers (Yang et al., 2007a,b; Schoups and Vrugt, 2010; Smith et al., 2010; Li et al., 2011) add a "gray box" before calculation of the likelihood function in the MCMC scheme.

The first-order autoregressive (AR(1)) scheme and the Box–Cox transformation method (BC) are widely used to remove errors' correlation and heteroscedasticity, respectively (Vrugt et al., 2009a; Schoups and Vrugt, 2010; Smith et al., 2010; Li et al., 2011). The Box–Cox transformation method needs to estimate transformation parameter (λ). Most studies (Vrugt et al., 2009a; Engeland et al., 2010; Li et al., 2011) fixed the value of λ, and some others (Yang et al., 2007a,b; Laloy et al., 2010) treat λ as an inference parameter. Obviously, it is more effective to remove the errors' heteroscedasticity when λ varied as model predictions. Unfortunately, almost all the inference results touch the boundary of $\lambda(0 \leqslant \lambda \leqslant 1)$, such as the result ($\lambda$) of Yang et al. (2007b) approaches to zero, and λ of Laloy et al. (2010) approaches to one. The boundary value means the extreme situation, e.g. when $\lambda = 1$, the BC is ineffective, i.e. no transformation of model residuals, and the BC becomes the log transformation when $\lambda = 0$, although it rarely occurs. Therefore, it is necessary to build a new efficient method to estimate the transformation parameter (λ) in the MCMC scheme.

Another question is: which probability distribution is appropriate for the random errors? Gaussian distribution is widely used as the probability distribution of the errors/residuals. However, recently some researchers have shown that there are many cases of non-Gaussian errors (Thiemann et al., 2001; Yang et al., 2007b; Schoups and Vrugt, 2010; Smith et al., 2010; Li et al., 2013). Some researchers proposed the Generalized Error Distribution (GED) (Thiemann et al., 2001; McMillan and Clark, 2009) and the Skew Generalized Error Distribution (SGED) (Schoups and Vrugt, 2010) that was developed from the GED.

The objective of this study is to assess the effect of different likelihood functions on the Bayesian inference in hydrological modeling. The primary goal is achieved through the following steps. Firstly, we establish a relationship between the Nash–Sutcliffe Efficiency coefficient (*NSE*) and the likelihood function; then we introduce a constraint to estimate the Box–Cox transformation (BC) parameter (λ); finally we compare three likelihood functions—*NSE*, Generalized Error Distribution with Box–Cox transformation (BC-GED) and Skew Generalized Error Distribution with Box–Cox transformation (BC-SGED) approaches—within the DiffeRential Evolution Adaptive Metropolis (DREAM) Markov Chain Monte Carlo (MCMC) scheme to discuss the effect of the form of likelihood function.

2. Study area and hydrologic model

2.1. Study area

The Baocun watershed (86.7 km^2) is a rural, mountainous watershed located in the eastern Jiaodong Peninsula in China (Fig. 1). The elevation of the watershed ranges from 20 m at the watershed outlet to about 220 m above mean sea level at the head-watershed. The length of the watershed is 16.1 km, the average width 5.4 km and the average slope 8.2‰. The climate of the watershed belongs to the Western Pacific Ocean extratropical monsoonal region with 70% of the rain falling between June and September (Fig. 2). The average annual precipitation is 805.6 mm with average annual potential evapotranspiration loss of 899.0 mm (measured by pan evaporation equipment termed E601). The average monthly temperature ranges from −0.8 °C in January to 24.4 °C in August. Fig. 2 shows that the warmest months correspond with the moistest months, and vice versa.

The geology of the watershed is mainly volcanic and metamorphic rocks, and the dominant parent materials of the soil are granite, diorite and gneiss. The dominant soil types are Luvisols, Regosols and Fluvisols covering about 94% of the area (FAO/IIASA/ISRIC/ISSCAS/JRC, 2009). The main land use is agriculture (terraced cropland), and the dominant crops are peanuts, corn and winter wheat. The agricultural lands are farmed three times every two years (termed crop rotation). The detailed schedules of planting crops are peanuts in May, winter wheat in October and corn in June next year.

2.2. SWAT-WB-VSA model

The Soil and Water Assessment Tool (SWAT) is popularly used for water resource management all over the world (Gassman et al., 2007). SWAT describes the spatial distribution of hydrological processes by dividing a watershed into multiple sub-basins, which are then further subdivided into hydrologic response units (HRUs) consisting of homogeneous land use, soil characteristics and slope. HRU is the smallest element of SWAT. The Soil Conservation Service curve number procedure (CN) is widely used to simulate the surface runoff generation in SWAT. However, the CN is an empirical method, which has some limitations in reflecting that soil moisture affects the surface runoff generation (Han et al., 2012). White et al. (2011) proposed a new model (termed SWAT-WB), which incorporated a physics-based rainfall-runoff approach (i.e. the Water Balance (WB) method) into SWAT. In this study, for reflecting the effect of topography on runoff, the Variable Source (runoff) Area (VSA) is incorporated into the SWAT-WB model. This new model is called SWAT-WB-VSA. In every HRU of