Bayesian forecasting and uncertainty quantifying of stream flows using Metropolis–Hastings Markov Chain Monte Carlo algorithm

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ABSTRACT

This paper presents a Bayesian approach using Metropolis–Hastings Markov Chain Monte Carlo algorithm and applies this method for daily river flow rate forecast and uncertainty quantification for Zhujiachuan River using data collected from Qiaotoubao Gage Station and other 13 gage stations in Zhujiachuan watershed in China. The proposed method is also compared with the conventional maximum likelihood estimation (MLE) for parameter estimation and quantification of associated uncertainties. While the Bayesian method performs similarly in estimating the mean value of daily flow rate, it performs over the conventional MLE method on uncertainty quantification, providing relatively narrower reliable interval than the MLE confidence interval and thus more precise estimation by using the related information from regional gage stations. The Bayesian MCMC method might be more favorable in the uncertainty analysis and risk management.

Key words: Bayesian approach; Metropolis–Hastings Markov Chain Monte Carlo algorithm; maximum likelihood estimation; uncertainty analysis

1 INTRODUCTION

Modeling hydrological processes including estimation of parameter associated with given model is an important issue in hydrological practice and water resources management. Two types modeling approach are typically used in hydrological modeling practice, i.e., Data driven modeling approach and mathematic modeling approach. Data driven modeling approach, also called statistic/stochastic approach, employs statistic or stochastic methods to study hydrological processes based on historical time series observation, e.g., river flow rate time series, without considering the detailed physical processes. Mathematic modeling approach usually solves a system of mathematic governing equations that represent the complex hydrological processes of being modeled at various levels of simplification accounting for the effect of other processes via parameters in the hydrological model.

Parameter estimation and uncertainty quantification are two crucial tasks in modeling practice including statistic modeling of hydrological processes where a probability density function (PDF) is usually selected to fit the historical hydrological data series, and further used for forecast purpose. Commonly used methods for parameter estimation include parametric methods such as method of moment, maximum likelihood estimation (MLE), weighted density method of moment, and least square method, and nonparametric methods such as kernel method. MLE is most commonly used due to its relatively higher accuracy and efficiency. Recently, some researchers have proposed the use of Bayesian approach for estimation of hydrological model parameters (Thiemann et al., 2001; Vrugt et al., 2003).

Modeling hydrological processes is always associated with unavoidable uncertainties from different component of model, including the simplification of hydrological process of concern by the selected model, model input, and uncertainties from the parameters in the selected model. Many efforts have been taken for quantification of the uncertainties from estimation of model parameters. Uncertainties are often estimated by confidence interval (Mishra, 2009; Smakhtin, 2001; Wang et al., 2009), which is based on asymptotic approximation quantify the lower bound and upper bound of modeling results given certain level of significance, usually 5% of significance.

However, such methods sometimes are unsatisfactory (Reis et al., 2005). An alternative approach to quantify uncertainties is based on a true posterior distribution using Bayesian approach that is further based upon the fundamental premise that all uncertainties must be represented by a probability distribution. Inferences about the primary variable of the model are described by a posterior distribution. The GLUE (generalized likelihood uncertainty estimation) approach (Beven and Binley, 1992) has been widely used for uncertainty analysis in hydrology during the past two decades. However, the calculating of a posterior distribution of the ordinary form is often very difficult when using Bayesian approach. This method therefore can only be used when there is a prior distribution of the conjugate (Vicens et al., 1975; Wood and Rodríguez-Iturbe, 1975). With the rapid advances in computing power and the rapid development of algorithms in recent years, many techniques have been proposed that provide estimates of the PDF of the model parameters as well as integrated uncertainty analysis for prediction through Monte Carlo simulations or

Markov-chain Monte Carlo (MCMC) schemes. With these advancements, using the Bayesian method for hydrological problems has become possible and practical (Zhang and Govindaraju 2000; Thiemann et al 2001; Wang 2001; O’Connell et al 2002; Vrugt et al 2003b; Reis et al 2005). Kuczera and Parent (1998) applied the Metropolis algorithm for assessment of parameter uncertainty in conceptual catchment models. Kuczera (1999) suggested calculating the expected PDF and confidence intervals using Monte Carlo-Bayesian methods. The study by O’Connell (2005) has shown that the use of paleo hydrologic information constraints can effectively reduce the uncertainty of flood frequency analysis. Parent and Bernier (2003) developed a Bayesian process to study annual peak flows using semi-conjugate priori information. Reis and Stedinger (2005) assessed the flood water level, the posterior distribution of flood risk, and the posterior distribution of the lognormal and Pearson type III curve parameter using Bayesian MCMC method. Bayesian method has also been applied to regional flood frequency (Gaume et al., 2010; Madsen and Rosbjerg, 1997; Reis and Stedinger, 2005). Using Bayesian MCMC approach, Lee and Kim (2008) identified uncertainty in regional low flow frequency and Kim and Lee (2010) analyzed the regional low flow frequency for a watershed in Korea.

This paper presents a Bayesian MCMC method using Metropolis–Hastings algorithm and applies this method for daily river flow rate forecast and uncertainty quantification for Zhujiachuan River based on daily flow rate data collected from Qiaotoubao Gage Station and other 13 gage stations in Zhujiachuan watershed in China. The proposed method is also compared with the conventional maximum likelihood estimation (MLE) for parameter

estimation and associated uncertainties. This paper is organized as follows. Section 2 details the Bayesian inference framework and Metropolis–Hastings algorithm and the MLE method. An application of the proposed approach is carried out and the estimated parameters are compared with MLE method in Section 3. The results are discussed and conclusions are summarized in Section 4.

2 METHODOLOGY

2.1 Bayesian theory

Classical statistical approach assumes that the parameters of a distribution are unknown but constant and identical to the parameters estimated from the sample statistics and the uncertainties of estimation are expressed using confidence intervals. Whereas, in Bayesian approach, the unknown parameters of a distribution including the primary parameter or variable of concern together with the parameters associated with the model are assumed to be random variables. In this way, uncertainty associated with the estimation of the parameters can be combined formally with the inherent variability of the primary random variable. The basic idea of Bayesian theory is to evaluate the background knowledge by analyzing the sample data, and to collect new data to improve the prior understanding. In a Bayesian model, a PDF is first assigned to the measured data set and unknown parameters, respectively, and then the joint PDF of all the random variables is obtained. Herein the total probability formula has been used that is given as

$$\pi(D, \theta) = L(D|\theta)\pi(\theta) \quad (1)$$

100 where $L(D|\theta)$ is the likelihood function and $\pi(\theta)$ is the prior distribution of random
 101 variable θ . For a random variable $\mathbf{X} = \{x_1, x_2, \dots, x_n\}$, the likelihood function $L(\theta)$ for the
 102 parameter vector θ associated with its PDF $f_X(x)$ is defined as

$$103 \quad L(\theta) = \prod_{i=1}^n f_X(x_i|\theta). \quad (2)$$

104 Given data D Bayesian theory can be used to determine the posterior distribution of θ .

$$105 \quad \pi(\theta|D) = \frac{L(D|\theta)\pi(\theta)}{\int L(D|\theta)\pi(\theta)d\theta} \quad (3)$$

106 where the denominator is the marginal distribution of data set. The posterior distribution
 107 $\pi(\theta|D)$ has collected the information on the prior distribution and current data, so that the
 108 parameter uncertainties are reduced.

109 The calculation of posterior distribution consists of three parts: (1) likelihood function;
 110 (2) prior distribution; and (3) marginal distribution. With given measurement data, all
 111 relevant measured information is already included in the likelihood function when making
 112 statistical inference to θ . Moreover, when two likelihood functions are proportional, the
 113 information they contain is same; this is called the *principle of the likelihood function*. For a
 114 measurement sample having measured values $x_1, x_2, \dots, x_n$, its likelihood function is the joint
 115 probability.

116 In the calculation of the posterior distribution, the most important part is the choice of
 117 the prior distribution. Selecting the prior distribution $\pi(\theta)$ needs to consider both the
 118 measured data and available prior knowledge. A prior distribution obtained from the existing

data and research results is called data-based prior distribution while non-data-based prior distribution refers to a prior distribution resulted from subjective judgments or theory. A special non-data-based prior distribution is no priori distribution, also called non-informative prior; in such case, the posterior distribution reflects data information only. Note that the denominator of Equation (3) is the marginal distribution that is a constant related only to the data set and irrelative to the parameters. For the marginal distribution, its analytic solution can be obtained only under very few special situations; in most cases, the marginal distribution has no analytical solution and is difficult to be obtained. This issue is also one of the disadvantages of Bayesian approach that actually has limited the application of Bayesian inference for a long time. Recently, MCMC methods have been used to avoid calculating the marginal distribution in Bayesian approach (Reis and Stedinger, 2005).

2.2 MCMC methods and Metropolis-Hastings algorithm

As discussed earlier, the calculation of the posterior distribution in implementing Bayesian theory is very difficult owing to the challenge of calculating the denominator of Equation (3). However, MCMC method can produce a sufficiently large number of samples from the posterior distribution function, which makes it possible to obtain precise nature of any desired posterior distribution. As a combination of Monte Carlo and Markov chain, MCMC method can be implemented by a variety of algorithms resulting in different Markov chains. Among them, Gibbs sampling method and Metropolis-Hastings (M-H) algorithm are the most commonly used two algorithms.

Metropolis-Hastings algorithm uses the Monte Carlo method to generate a data set that converges to the target PDF, in other words, the basic idea of Metropolis-Hastings is to construct a Markov chain with an invariant target distribution. In order to estimate this target distribution function $\pi(\theta|D)$, M-H algorithm needs an auxiliary PDF $q(x, y)$ generally called proposal function or proposal distribution. A proposal function needs to meet three requirements, (1) $q(y|x)$ is a PDF; (2) $q(x, y)$ can be calculated; and (3) Random numbers can be easily generated from $q(x, y)$. Among the three requirements, $q(x, y)$ could be arbitrarily selected. After $q(x, y)$ is selected, the M-H algorithm can be illustrated as the following steps:

- i) Set an arbitrary starting point θ_0 for calculation at $i = 0$;
- ii) Generate a new value θ_* from the proposal function $q(x, y)$;
- iii) Calculate the probability of acceptance

$$\rho(\theta_i, \theta_*) = \min \left[\frac{q(\theta_i|\theta_*)\pi(\theta_*|D)}{q(\theta_*|\theta_i)\pi(\theta_i|D)}, 1 \right] \quad (4)$$

- iv) Generate a random number u from uniform distribution $[0, 1]$;
- v) If $u < \rho$, then set $\theta_{i+1} = \theta_*$; otherwise set $\theta_{i+1} = \theta_i$ and $i = i + 1$, and return to Step ii.

Reis and Stedinger (2005) pointed out that although theoretically the proposal function $q(x, y)$ can be arbitrarily selected, in practice the selection of $q(x, y)$ influence the efficiency of computation significantly. They used normal and gamma distribution as

proposal functions in their study. Chib and Greenberg (1995) reviewed five families of distribution for candidate proposal function and recommend to try a different family of candidate-generating PDF if the generated chain with the "optimal" acceptance rate still displays high autocorrelations .

Normal distribution is probably the most commonly used proposal function. In this way, $q(x, y)$ is not only symmetry, but only related to $x - y$. In other words, $q(\theta_i | \theta_j) = q(\theta_j | \theta_i)$. Equation (4) can then be simplified as

$$\rho(\theta_i, \theta_*) = \min \left[\frac{\pi(\theta_* | D)}{\pi(\theta_i | D)}, 1 \right] \quad (5)$$

It should be noted that in Equation (5) only the ratio of posterior distribution rather than the posterior distribution is calculated. As discussed earlier, while the denominator of the posterior distribution is difficult to calculate, it is an integral of the marginal distribution, irrelevant to θ .

By calculating Equation **Error! Reference source not found.**, the Metropolis-Hastings algorithm can avoid the difficulty of calculating the denominator of the posterior distribution in Bayesian theorem.

Another issue when using the Metropolis-Hastings algorithm is the efficiency of the algorithm. This can be measured in terms of the acceptance rate. A very low acceptance rate indicates that the generated random number by the algorithm is far away from the target distribution and the algorithm is thus invalid. If the acceptance rate is too high, it may take long time to generate data that fit the target distribution, and the algorithm is therefore invalid

as well. Accounting for both the efficiency and quality of the generated data, Roberts et al. (1997) proposed the most appropriate acceptance rate 0.45 for single parameter estimation and 0.23 for multiple parameter estimation. Gamerman (1997) suggests that the acceptance rate between 0.2 to 0.5 is acceptable.

2.3 Maximum likelihood estimation (MLE)

MLE method together with the method of moment is a major standard method in statistical inference. This method is consistent, asymptotically normal and efficient under some regularity conditions according to the theory of ML. For a random variable $\mathbf{X} = \{x_1, x_2, \dots, x_n\}$, the likelihood function $L(\theta)$ for the parameters vector θ associated with PDF $f_X(x)$ is defined as $L(\theta) = \prod_{i=1}^n f_X(x_i|\theta)$. The MLE is to obtain the estimate of θ , namely $\hat{\theta}$ by maximizing the likelihood function given the data set.

$$\hat{\theta} = \operatorname{argmax} L(\theta) \quad (6)$$

Equation (6) can be solved by multiple times of differentiating $L(\theta)$ and let each differential equal to zero. In practice, only m times of differentiation are needed in order to solve m parameters of θ .

In addition to being used for parameter estimate, MLE has also been applied to quantify the uncertainties in parameter estimation. Under the assumption of normality and linearity, the uncertainty of parameter is obtained through quadratic approximation of the likelihood ratio or the Fisher information matrix. The likelihood ratio can be approximated as

$$\log RL(D|\theta) = \log \frac{L(D|\theta)}{L(D|\hat{\theta})} \cong a + b\theta + c\theta^2. \quad (7)$$

where $\hat{\theta}$ is estimation of parameter θ . Equation (7) needs to satisfy some conditions, including 1) the right hand side reaches the maximum at $\theta = \hat{\theta}$, and 2) its maximum value should be zero. It therefore can be rewritten as

$$\log RL(D|\theta) = \log \frac{L(D|\theta)}{L(D|\hat{\theta})} \cong -\frac{1}{2} I (\theta - \hat{\theta})^2 \quad (8)$$

where I is a positive constant also known as the expected information. Following Meeker and Escobar (1998) with assumption of normality, the estimated parameter by MLE is given as

$$\hat{\theta} = \theta + \frac{1}{I} \frac{\partial \log L}{\partial \theta} \quad (9)$$

and the asymptotic distribution of MLE is

$$\hat{\theta} \sim N(\theta, I^{-1}) \quad (10)$$

which can be standardized as

$$\frac{\hat{\theta} - \theta}{\sqrt{1/I}} = \sqrt{I} (\hat{\theta} - \theta) \sim N(0,1) \quad (11)$$

Given one tail normal quantile $z_{(1-\alpha/2)}$ at the significance level α ,

$$\Pr \left[\sqrt{I} (\hat{\theta} - \theta) > z_{(1-\alpha/2)} \right] = \alpha / 2 \quad (12)$$

or both side tail confidence interval,

$$\Pr \left[\left| \sqrt{I} (\hat{\theta} - \theta) \right| \leq z_{(1-\alpha/2)} \right] = 1 - 2(\alpha / 2) = 1 - \alpha \quad (13)$$

212 The range of parameter θ corresponding to $\left| \sqrt{I}(\hat{\theta} - \theta) \right| \leq z_{(1-\alpha/2)}$ is

$$213 \quad \hat{\theta} - \frac{z_{(1-\alpha/2)}}{\sqrt{I}} \leq \theta \leq \hat{\theta} + \frac{z_{(1-\alpha/2)}}{\sqrt{I}} \quad (14)$$

214 where $\sqrt{I}$ can be obtained by calculating the standard deviation of the sample data. It has
215 been reported that this approximation method is very effective for a large sample, but less
216 effective when a small number of samples are used (Bickel and Doksum, 1977).

217 **3 BAYESIAN UNCERTAINTY QUANTIFYING AND** 218 **FORECASTING OF STREAM FLOWS USING** 219 **METROPOLIS–HASTINGS ALGORITHM**

220 In this study, we apply the proposed Bayesian MCMC method to analyze the uncertainties of
221 the daily flow rate, and predict the 1987 daily flow rate, of Qiaotoubao gage station (also
222 called Qiaotou gage station), based on the 1956-1986 historical daily flow rates of 14 gage
223 stations in Zhujiachuan watershed, a watershed in Yellow River basin in China. For
224 illustration purpose, we present in detail the uncertainties quantification for the January 31
225 flow rates of Qiaotoubao gage station using Bayesian MCMC method in this section, based
226 on the historical January 31 daily flow rates (1956 to 1986) of the 13 gaging stations in
227 Zhujiacha watershed. The same procedure is followed to quantify the uncertainties of flow
228 rate for the other calendar days of the whole year, for instance, the flow rates of February 1,
229 based on the corresponding historical daily flow rates of that calendar day, for instance, the
230 flow rates of February 1, 1956-1986.

3.1 Study area and data

The Zhujiachuan River is a tributary of Yellow River, originated from Shuo County, Shanxi Province, China. It flows through Wuzhai County, Hequ County, Baode County, and eventually into Yellow River. The average annual flow of Zhujia River is 145.6 million m^3 , with average flow rate $1.78 \text{ m}^3/\text{s}$ and peak flow rate of $2000 \text{ m}^3/\text{s}$ during flooding season. The river is 167.6 km long and the watershed area is 2901 km^2 . Qiaotoubao Gage Station is a major gage station in Zhujiachuan River, located in 111.13°E , 38.93°N . There are 13 other gaging stations in the watershed which are shown in Figure 1. The daily flow rates from 1956 – 1986 at Qiaotoubao Gage Station as well as the other 13 gage stations in the Zhujiachuan watershed are collected for this study. The January 31 daily flow rate data (1956 - 1986) of Qiaotoubao Gage Station are plotted in Figure 2, and some descriptive statistics for the data is given in Table 1. The daily flow rate varies from $3.11 \text{ m}^3/\text{s}$ occurring in 1981 to $10.76 \text{ m}^3/\text{s}$ appearing in 1959; the mean daily flow rate is $5.91 \text{ m}^3/\text{s}$ with a variance of $3.25 \text{ m}^3/\text{s}$.

3.2 The prior distribution and proposal function

The first task would be determining the prior distribution of flow rate. This study uses a priori distribution function that is based on the regional information data, i.e., from the 13 gage stations in Zhujiachuan watershed. The Kolmogorov–Smirnov (K-S) test is performed to identify the distribution of the January 31 daily flow data (1956-1987), and the distributions of its associated parameters. The K-S test results are presented in Table 2 which indicates that the daily flow rates of January 31, 1956-1986 follow the two-parameter

249 Weibull distribution at the significance level of 0.05. The PDF and CDF of Weibull
 250 distribution are given as

$$\begin{aligned}
 f(x) &= \frac{\alpha}{\beta} \left(\frac{x}{\beta} \right)^{\alpha-1} \exp \left[- \left(\frac{x}{\beta} \right)^{\alpha} \right] \\
 F(x) &= 1 - \exp \left[- \left(\frac{x}{\beta} \right)^{\alpha} \right]
 \end{aligned}
 \tag{15}$$

252 where α and β are shape parameter and scale parameter, respectively. The CDF of the flow
 253 rate data is plotted in Figure 3 (Upper).

254 Given the Weibull distribution of flow rate data, its likelihood function can be
 255 obtained

$$L(D|\theta) = L(D|\alpha, \beta) = \left(\frac{\alpha}{\beta} \right)^n \prod_{i=1}^n \left(\frac{x_i}{\beta} \right)^{\alpha-1} \exp \left[- \left(\sum_{i=1}^n \left(\frac{x_i}{\beta} \right)^{\alpha} \right) \right]
 \tag{16}$$

257 The next task would be identifying the distribution of parameters α and β in the
 258 Weibull distribution. K-S test is performed for the daily flow rates of January 31, 1956
 259 through 1986; and the teste indicates that Weibull distribution fits the flow rate data in each
 260 of the 13 gage stations. The parameters of parameters α and β associated with Weibull
 261 distribution of flow rate data of each gage station are then estimated. The K-S test is
 262 performed again to the estimated 14 α and β data (one for Qitaotoubao gage station and 13
 263 for the other 13 gage stations in Zhujiachuan watershed). It shows that the parameters α and
 264 β also follow Weibull distribution, as shown in Table 2 and Figure 3 (Middle) and (Lower)
 265 respectively.

266 The PDFs of parameters α and β are given respectively as

$$\begin{aligned}\pi(\alpha) &= \frac{b_1}{a_1} \left(\frac{\alpha}{a_1} \right)^{b_1-1} \exp \left(- \left(\frac{\alpha}{a_1} \right)^{b_1} \right) \\ \pi(\beta) &= \frac{b_2}{a_2} \left(\frac{\beta}{a_2} \right)^{b_2-1} \exp \left(- \left(\frac{\beta}{a_2} \right)^{b_2} \right)\end{aligned}\tag{17}$$

where $a_1 = 8.1361$, $b_1 = 0.8815$, $a_2 = 3.6525$, and $b_2 = 2.5669$, all being the parameters of the prior distribution. Assume α and β are statistically independent, then

$$\pi(\theta) = \pi(\alpha, \beta) = \frac{b_1 b_2}{a_1 a_2} \left(\frac{\alpha}{a_1} \right)^{b_1-1} \left(\frac{\beta}{a_2} \right)^{b_2-1} \exp \left(- \left(\frac{\alpha}{a_1} \right)^{b_1} - \left(\frac{\beta}{a_2} \right)^{b_2} \right).\tag{18}$$

All the prior distributions are so far obtained.

As addressed in the section of Metropolis-Hastings algorithm, Normal distribution is adopted as the proposal function in this study. Selection of the proposal distribution function is critical to the efficiency of Metropolis-Hastings algorithm, which can be measured by the acceptance rate. In this study, Equation (5) can be further written as

$$\rho(\theta_i, \theta_*) = \min \left[\frac{L(D|\alpha_*, \beta_*) \pi(\alpha_*, \beta_*)}{L(D|\alpha_i, \beta_i) \pi(\alpha_i, \beta_i)}, 1 \right]\tag{19}$$

Either a too low or too high acceptance rate indicates the M-H algorithm is invalid. The parameters of α and β are respectively given in the last row of Table 3 α section and β section, and their corresponding acceptance rates are 0.418 and 0.422, respectively, indicating the M-H algorithm in this study is satisfactory. 100,000 samples are generated for the simulation of each parameter using Metropolis-Hastings algorithm.

3.3 Comparison between Bayesian MCMC estimation and MLE

We compare the Bayesian MCMC method and MLE method for uncertainty analysis for the flow rate of January 31 (1956-1986) at in Qiaotoubao Gage Station following Lee and Kim (2008). We first compare Bayesian MCMC method and MLE method on uncertainty analysis of parameters α and β using eight synthetic sets of α and β around the estimated parameters $\alpha = 6.5295$ and $\beta = 3.4761$, which are presented in Column 1 of Table 3. Using Weibull distribution with the “true” values of each set of α and β , 31 samples representing the 31-year (1958-1986) flow rates of January 31 at Qiaotoubao Gage Station are generated for each set of α and β . MLE method and Bayesian MCMC approach using the prior distribution given by Equation (18) and the likelihood function given by Equation (16) are then used to estimate the parameters. Note that the eighth pairs of α and β are actually the estimated parameters from the observation flow rates data series.

The estimation results for α and β by MLE and Bayesian MCMC method using Metropolis-Hastings algorithm are given in Table 3. The discrepancies between estimated mean value and the “true” value of α by either method is about within 3%, except for the estimated α for the case of α with “true” value of 14.0 by MLE where estimated mean value is about 6% larger than the “true” value. The estimations of α by the two methods are very close, with small differences varying from 0.039 to 1.430 (as shown in the last column of Table 3). Similarly, The discrepancies between estimated mean value and the “true” value of β by either method is about within 2-3% and the differences of estimated mean value of β by the two methods vary from 0.005 to 0.207 (as shown in the last column of Table 3).

Compared with the corresponding “true” values of α and β , these results indicate that the Bayesian MCMC methods and MLE method perform closely on the estimation of mean α and β values. However, the confidence intervals by the MLE and Bayesian MCMC method (also known as a “credible interval”) show significant difference, as shown in Table 3 and Figure 4. The width between the upper and lower bound of credible interval of estimated α ranges from 1.120 to 1.403 with Bayesian MCMC method, but the MLE confidence interval varies from 1.027 to 5.570. The width between the upper and lower bound of reliable interval of estimated β ranges from 0.265 to 0.673 in Bayesian MCMC method, but the confidence interval varies from 0.813 to 1.504 in MLE method. The relatively narrower width of reliable interval implies that Bayesian MCMC method performs over the MLE method in quantification of uncertainty. Figure 4 plots the 95% reliable intervals estimated by Bayesian MCMC method and the 95% confidence intervals by MLE; the one estimated by Bayesian MCMC method is clearly narrow than those estimated by MLE method. For example, for the 95% confidence interval estimated by MLE method for $\beta = 2.5$ is [2.1384, 2.9509], much wider than the counterpart by Bayesian MCMC method, [1.5393, 2.6851].

The estimated PDF for the daily flow rates of January 31 (1956-1986) by MLE and Bayesian MCMC method based on the observation data are plotted in Figure 5. Similar to the case of estimation of parameters for α and β , the PDF of the flow rates of January 31 at 95% confidence level estimated by Bayesian MCMC method is within a narrower range than those estimated by MLE method (Gaume et al., 2010; Kim and Lee, 2010; Lee and Kim, 2008). The smaller deviations shown in Figure 5 indicate the Bayesian MCMC method performs

over MLE on uncertainty quantification. This is understandable in that MLE method uses Equation (14) to estimate the confidence interval, and these equations are approximately precise only when a large number of normally distributed samples are available. However, in this study this assumption does not hold well with only 31 years of samples, thus resulting in unsatisfactory estimation by MLE.

3.4 Daily flow rate prediction and uncertainty quantification

The present Bayesian MCMC method using M-H algorithm is also applied to predict the flow rates for 1987. For illustration purpose, we present in detail the calculation of the daily flow rate of January 31, 1987 based on the observation flow rates of January 31, 1958 through 1986. The predicted flow rate of January 31, 1987 is 3.64, 4.58, and 5.53 m³/s at 2.5%, 50%, and 97.5% probability, respectively. Compared with the observation flow rate of January 31, 1987, 4.12 m³/s, the predicted flow rate and estimated credible intervals are satisfactory. Following the same process for forecasting the flow rate of January 31, 1987 at Qiaotaobao Gage Station using Bayesian MCMC method, we can obtain the predicted flow rates of each calendar day of 1987, as plotted in Figure 6 (Upper).

Figure 6 (Upper) shows that while the forecasts are very close to the observation data in most period of forecast except some days between May and August, all the observed flow rates in the forecast period are within the 95% credible intervals, indicating a good performance of Bayesian MCMC method in prediction and uncertainty quantification. While Figure 6 (Upper) shows that the predicted daily flow rates match the observations very well, Figure 6 (Lower) depicts the 95% credible interval of the estimations is relatively narrow in

the period of November through March. The discrepancies between forecast values and observations become a little larger and the 95% credible interval become a little wider in April, remains in a relatively wider range from May to August, and narrows down again after August. The widest credible interval occurs on August 7, 1987, being $115\text{m}^3/\text{s}$.

Figure 6 (Lower) plots the predicted mean daily flow rate and the 95% credible interval. It shows that the mean daily flow rates are larger than the corresponding 95% credible intervals in September through April, owing to the relatively small variation (annual variation) of daily flow rate in this period. From May to August, the predicted mean flow rates are close to the 95% credible intervals, due to the relatively large variation of daily flow rates. It is also noticed that the 95% credible intervals become wider as the daily flow rates increase, indicating a relatively large uncertainty compared with the low flow periods. From the perspective of uncertainty, the prediction uncertainty is small in the period of September through April, as the daily flow rates are relative stationary. When the flow rates vary in a relatively wider range during May to August, the associated prediction uncertainty becomes larger.

4 DISCUSSION AND CONCLUSION

This paper presents a Bayesian MCMC method using M-H algorithm for daily flow rate forecast and the associated uncertainty quantification. This approach is completely based on the posterior distribution function and there are no approximation steps in anywhere of the theoretical framework, making the prediction more precise.

The proposed method is compared with the conventional MLE method through the estimation of parameters in the case study of daily flow rate analysis for Zhujiachuan River in China based on the historical observation data at Qiaotoubao Gage Station and 13 other gage stations in the Zhujiachuan watershed. Compared with the conventional MLE method, while the Bayesian MCMC performs similarly on estimating the mean value of daily flow rate, it performs over the MLE method on uncertainty quantification (Gaume et al., 2010; Kim and Lee, 2010; Lee and Kim, 2008), providing relatively narrower credible interval and thus more precise estimation by using the related information from regional gage stations. The Bayesian MCMC method, therefore, is more favorable for the uncertainty analysis and risk management.

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REFERENCE

Beven, K., Binley, A., 1992. The future of distributed models: model calibration and

uncertainty prediction. *Hydrol. Process.* 6, 279–298. doi:10.1002/hyp.3360060305

Bickel, P.J., Doksum, K.A., 1977. *Mathematical Statistics: Basic Ideas and Selected Topics*. Holden-Day, San Francisco.

Chib, S., Greenberg, E., 1995. Understanding the metropolis-hastings algorithm. *Am. Stat.* 49, 327–335.

Coles, S.G., Powell, E.A., 1996. Bayesian methods in extreme value modelling: a review and new developments. *Int. Stat. Rev. Int. Stat.* 119–136.

Gamerman, D., 1997. *Markov chain Monte Carlo: stochastic simulation for Bayesian inference*. Chapman Hall, London.

Gaume, E., Gaál, L., Viglione, A., Szolgay, J., Kohnová, S., Blöschl, G., 2010. Bayesian MCMC approach to regional flood frequency analyses involving extraordinary flood events at ungauged sites. *J. Hydrol.* 394, 101–117. doi:10.1016/j.jhydrol.2010.01.008

Kelly, K.S., Krzysztofowicz, R., 1994. Probability distributions for flood warning systems. *Water Resour. Res.* 30, 1145–1152.

Kim, S.U., Lee, K.S., 2010. Regional low flow frequency analysis using Bayesian regression and prediction at ungauged catchment in Korea. *KSCE J. Civ. Eng.* 14, 87–98. doi:10.1007/s12205-010-0087-7

Krzysztofowicz, R., 1999. Bayesian theory of probabilistic forecasting via deterministic hydrologic model. *Water Resour. Res.* 35, 2739–2750.

Krzysztofowicz, R., 1983. A Bayesian Markov model of the flood forecast process. *Water Resour. Res.* 19, 1455–1465.

Kuczera, G., 1999. Comprehensive at-site flood frequency analysis using Monte Carlo Bayesian inference. *Water Resour. Res.* 35, 1551–1557.

Kuczera, G., Parent, E., 1998. Monte Carlo assessment of parameter uncertainty in conceptual catchment models: the Metropolis algorithm. *J. Hydrol.* 211, 69–85.

Lee, K.S., Kim, S.U., 2008. Identification of uncertainty in low flow frequency analysis using Bayesian MCMC method. *Hydrol. Process.* 22, 1949–1964. doi:10.1002/hyp.6778

Madsen, H., Rosbjerg, D., 1997. Generalized least squares and empirical bayes estimation in regional partial duration series index-flood modeling. *Water Resour. Res.* 33, 771–781.

Madsen, H., Rosbjerg, D., Harremoës, P., 1994. PDS-modelling and regional Bayesian estimation of extreme rainfalls. *Nord. Hydrol.* 25, 279–300.

Meeker, W.Q., Escobar, L.A., 1998. *Statistical Methods for Reliability Data*. Wiley, New York.

Mishra, S., 2009. Uncertainty and sensitivity analysis techniques for hydrologic modeling. *J. Hydroinformatics* 11, 282.

- O'Connell, D.R.H., 2005. Nonparametric Bayesian flood frequency estimation. *J. Hydrol.* 313, 79–96.
- O'Connell, D.R.H., Ostenaar, D.A., Levish, D.R., Klinger, R.E., 2002. Bayesian flood frequency analysis with paleohydrologic bound data. *Water Resour. Res.* 38, 11–16.
- Parent, E., Bernier, J., 2003. Bayesian POT modeling for historical data. *J. Hydrol.* 274, 95–108.
- Reis, D.S., Stedinger, J.R., 2005. Bayesian MCMC flood frequency analysis with historical information. *J. Hydrol.* 313, 97–116. doi:10.1016/j.jhydrol.2005.02.028
- Reis, D.S., Stedinger, J.R., Martins, E.S., 2005. Bayesian generalized least squares regression with application to log Pearson type 3 regional skew estimation. *Water Resour. Res.* 41.
- Roberts, G.O., Gelman, A., Gilks, W.R., 1997. Weak convergence and optimal scaling of random walk Metropolis algorithms. *Ann. Appl. Probab.* 7, 110–120.
- Smakhtin, V.U., 2001. Low flow hydrology: A review. *J. Hydrol.*
- Thiemann, M., Trosset, M., Gupta, H., Sorooshian, S., 2001. Bayesian recursive parameter estimation for hydrologic models. *Water Resour. Res.* 37, 2521–2535.
- Vicens, G.J., Rodríguez-Iturbe, I., Schaake, J.C., 1975. A Bayesian framework for the use of regional information in hydrology. *Water Resour. Res.* 11, 405–414. doi:10.1029/WR011i003p00405
- Vrugt, J.A., Gupta, H. V, Bouten, W., Sorooshian, S., 2003. A Shuffled Complex Evolution Metropolis algorithm for optimization and uncertainty assessment of hydrologic model parameters. *Water Resour. Res.* 39.
- Wang, H., Lin, X., Qian, L., 2009. Cryptic period analysis model of hydrological process and its application. *Hydrol. Process.* 23, 1834–1843. doi:10.1002/hyp.7313
- Wang, Q.J., 2001. A Bayesian joint probability approach for flood record augmentation. *Water Resour. Res.* 37, 1707–1712.
- Wood, E.F., Rodríguez-Iturbe, I., 1975. Bayesian inference and decision making for extreme hydrologic events. *Water Resour. Res.* 11, 533–542.
- Zhang, B., Govindaraju, R.S., 2000. Prediction of watershed runoff using Bayesian concepts and modular neural networks. *Water Resour. Res.* 36, 753–762.

Table 1. Descriptive statistics of January 31 (1956-1986) daily flow rate data

Mean	5.91
Standard Error	0.32
Median	5.62
Standard Deviation	1.80
Sample Variance	3.25
Kurtosis	0.31
Skewness	0.68

Table 2. K-S test results of prior distribution for January 31 (1956-1986) flow rates and the prior distribution of its associated parameters

Hypothesis test result	P	K-S test statistic	Critical value
January 31 flow rates of Qiaotaobao Gage Station n			
0	0.7765	0.1136	0.2346
Parameter α			
0	0.8858	0.1497	0.3489
Parameter β			
0	0.5610	0.2930	0.3219

Note: The null hypothesis of K-S test in this study is that the data follows Weibull distribution. The test result 0 means that the null hypothesis of K-S test is not rejected. Critical value is the K-S statistics at P value of 0.05.

Table 3. Comparison of Bayesian MCMC with MLE for estimation of α and β

	MLE				Bayesian MCMC				Diff. of Mean (f)-(c)
	2.50% (a)	50% (b)	97.50% (c)	Diff. (c)-(a)	2.50% (e)	50% (f)	97.50% (g)	Diff. (g)-(e)	
α									
2.0000	1.4551	1.9685	2.4819	1.0268	1.5393	2.0519	2.6851	1.1458	0.0834
4.0000	3.0109	3.9507	4.8905	1.8796	3.5534	4.1332	4.7690	1.2156	0.1825
6.0000	4.1830	5.6312	7.0795	2.8965	5.6720	6.2352	6.8755	1.2035	0.6040
8.0000	6.2436	7.9220	9.6004	3.3568	7.0372	7.6693	8.3397	1.3025	0.2527
10.0000	7.9931	10.0494	12.1057	4.1126	9.4405	10.0883	10.7620	1.3215	0.0390
12.0000	9.6735	12.1574	14.6413	4.9678	11.5203	12.1189	12.8992	1.3789	0.0385
14.0000	12.0571	14.8420	17.6269	5.5698	12.7906	13.4121	14.1932	1.4026	1.4299
6.5295	5.0392	6.4340	7.8288	2.7896	5.8153	6.3276	6.9349	1.1196	0.1064
β									
2.5000	2.1384	2.5446	2.9509	0.8125	2.4244	2.5396	2.6897	0.2653	0.0050
3.0000	2.6392	3.1120	3.5848	0.9456	2.7878	2.9456	3.1226	0.3348	0.1664
3.5000	3.1134	3.6066	4.0997	0.9863	3.3152	3.4972	3.7214	0.4062	0.1094
4.0000	3.4885	4.0963	4.7041	1.2156	3.7555	3.9920	4.2542	0.4987	0.1043
4.5000	3.8153	4.5076	5.1998	1.3845	4.2437	4.5000	4.8069	0.5632	0.0076
5.0000	4.5393	5.1411	5.7429	1.2036	4.6583	4.9338	5.2482	0.5899	0.2073
5.5000	4.8786	5.6304	6.3821	1.5035	5.4355	5.7509	6.1087	0.6732	0.1206
3.4761	2.8051	3.4391	4.0731	1.2680	3.2834	3.4047	3.6090	0.3256	0.0344

Figure 1. Sketch map of study area Zhujiachuan watershed

Figure 2. January 31 daily flow rates (1955-1986) of Zhijiachuan River at Qiaotoubao Gage Station

Figure 3. Empirical distribution of parameters against Weibull distribution.
Upper: X-axis represents Flow rate of January 31, 1956-1986, (m^3/s); Middle: X-axis is value of α ; Lower: X-axis is β

Figure 4. Uncertainty analysis for α (Upper) and β (Lower).
Each circle corresponds to an α (Upper) and β (Lower) point in Table 3.

Figure 5. PDF of flow rate of January 31 (1956-1986). Upper: by MLE; Lower: by Bayesian MCMC

Figure 6. Bayesian MCMC prediction of 1987 flow rate at Qiaotoubao Gage Station.
Upper: Bayesian MCMC prediction and 95% confidence interval; Lower: Bayesian MCMC prediction and 95% confidence interval width

Schematic diagram of study area

Figure 1 Sketch of study area Zhujiachuan watershed

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