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Precipitation estimation and error reconstruction from an ensemble of hydrologic models

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Precipitation estimation and error reconstruction from an ensemble of hydrologic models

THESIS

submitted in partial satisfaction of the requirements
for the degree of

MASTER OF SCIENCE

in Environmental Engineering

by

Hao Guo

Thesis Committee:
Assistant Professor Jasper A. Vrugt, Chair
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ABSTRACT OF THE THESIS

Precipitation estimation and error reconstruction from an ensemble of hydrologic models

By

Hao Guo

Master of Science in Environmental Engineering

University of California, Irvine, 2015

Assistant Professor Jasper A. Vrugt, Chair

Bayesian methods are finding increasing application and use in environmental modeling. Bayes law states that the posterior, $P(\boldsymbol{\theta}|\tilde{\mathbf{D}})$ is proportional to the product of the prior, $P(\boldsymbol{\theta})$ and likelihood, $L(\boldsymbol{\theta}|\tilde{\mathbf{D}})$, or in mathematical form, $P(\boldsymbol{\theta}|\tilde{\mathbf{D}}) \propto P(\boldsymbol{\theta})L(\boldsymbol{\theta}|\tilde{\mathbf{D}})$. The main crux in the application of such methods relies in the definition of the likelihood function, $L(\boldsymbol{\theta}|\tilde{\mathbf{D}})$ used to summarize the distance between the n model simulated values, $\mathbf{D}$ and corresponding data, $\tilde{\mathbf{D}}$. Under ideal conditions, the residuals exhibit normality and standard likelihood functions will suffice. Yet, in real-world modeling studies the residuals are dominated by model and input data errors with probabilistic properties that are not easy to capture in the construction of a likelihood function. Recent contributions therefore use latent variables to parameterize model input and structural errors and estimate these variables jointly with the model parameters, $\boldsymbol{\theta}$. We caution against this approach in the present thesis and demonstrate that the posterior values of the latent variables strongly depend on the (hydrologic) model structure being used. Although strong priors can be used to somewhat alleviate this problem, this requires explicit information about the size and space/time correlation of the input data errors. An alternative viewpoint emerges that model structural errors are relative and only meaningfully interpreted on a model comparative basis.

Chapter 1

Introduction

The movement of water through watersheds is an incredibly complex process that is controlled by a myriad of processes and properties that interact and exhibit large spatial and temporal variations. Despite significant advances in remote sensing and in-situ measurement technologies, available data is often of insufficient resolution to warrant an accurate characterization of (amongst others) small-scale variability in topography, subsurface flow and transport properties, vegetation, soil types, flow paths, and forcing conditions deemed necessary for detailed distributed simulation of soil moisture flow, groundwater recharge, surface runoff, preferential flow, root water uptake, and river discharge. This lack of high resolution and high quality data faces hydrologists with tremendous challenges, and forces hydrologic modelers to describe spatially distributed vegetation and subsurface properties with much simpler homogeneous units using transfer functions that describe the flow of water within and between different storage compartments. A consequence of this aggregation process is that most of the parameters in hydrologic models cannot be inferred through direct observation in the field, but can only be meaningfully derived by calibration against an input-output record of the catchment response. In this process the parameters are adjusted in such a way that the model approximates as closely and consistently as possible the response of the catchment over some historical period of time. The parameters estimated in this manner represent effective conceptual representations of spatially and temporally heterogeneous watershed properties.

During the past four decades much research has been devoted to the development of computer based methods for fitting hydrologic models to data (e.g. streamflow, water chemistry, groundwater table depth, soil moisture, pressure head, snow water equivalent). That research has primarily focused on six different issues: (1) the development of specialized objective functions that appropriately represent and summarize the errors between model predictions and observations, (2) the search for efficient optimization algorithms that can reliably solve the hydrologic model calibration problem, (3) the determination of the appropriate quantity and most informative kind of data, (4) the selection of an appropriate numerical solver for the partially structured differential and algebraic equation systems of hydrologic models, (5) the representation of uncertainty, and (6) the development of methods for inferring and refining the mathematical structure and process equations of hydrologic models.

Research into error residual distributions had led to the development of a suite of different (hierarchical) likelihood functions for measuring the "closeness" between the model simulations (predictions) and the corresponding data (*Ibbitt and O'Donnell*, 1974; *Sorooshian and Dracup*, 1980; *Kuczera*, 1983a; *Bates and Campbell*, 2001; *Kavetski*, 2006a; *Marshall et al.*, 2007; *Schoups and Vrugt*, 2010a; *Smith et al.*, 2010). Recent work by *Schoups and Vrugt* (2010a) has resulted in a generalized likelihood function that encapsulates many of the existing likelihood functions in the hydrologic literature, but with additional flexibility to simultaneously account for correlated, heteroscedastic, and nontraditional error residual distributions.

Research into optimization methods has led to the development of a wide variety of different search methods. Whereas initial approaches utilized local search principles that seek iterative improvement of the objective function from a single starting point in the parameter space (*Ibbitt*, 1972; *Johnston and Pilgrim*, 1976; *Sorooshian and Dracup*, 1980; *Restrepo*, 1982; *Kuczera*, 1983a,b; *Gupta and Sorooshian*, 1983; *Sorooshian et al.*, 1983b; *Troutman*, 1985a,b), problems with parameter insensitivity, curved ridges, local minima, and multiple different regions of attraction has stimulated the development of population based search algorithms that use multiple different points concurrently to locate the global optimum *Wang* (1991); *Duan et al.* (1992); *Yapo et al.* (1998); *Seibert* (2000); *Vrugt et al.* (2003b); *Khu and Madsen* (2005); *Chu et al.* (2010). In this regard, the Shuffled Complex Evolution global optimization algorithm of *Duan et al.* (1992) has shown to be effective and efficient in calibrating conceptual watershed models. Recent developments include simple randomized adaptation (*Mazi et al.*, 2004; *Tolson and Shoemaker*, 2007), multimethod ensemble (*Vrugt and Robinson*, 2007a; *Vrugt et al.*, 2008b), and filtering based (*Pauwels*, 2008) parameter estimation methods that further improve search efficiency and reliability.

Research into the information content of data has led to the understanding that it is not the length of the data that matters, but the variability of the observed discharge data (*Kuczera*, 1982; *Sorooshian et al.*, 1983a; *Gupta and Sorooshian*, 1985; *Yapo et al.*, 1996; *Vrugt et al.*, 2006c). Wet and dry periods are both required to make sure that all the different components of the watershed model are excited and the different parameters can be estimated from the calibration data. Post-audit simulations presented in *Vrugt et al.* (2002) using a Bayesian analysis, adaptive Random Walk Metropolis resampling, and value of information (VOI) framework has demonstrated that only a few (daily) streamflow data measurements are necessary to reliably calibrate a conceptual hydrologic model. The remaining data contain redundant information and cannot be used to evaluate the adequacy of the actual model structure.

Research into numerical solvers has demonstrated that explicit (Euler based) time-stepping schemes introduce considerable streamflow simulation errors and spurious local minima, pits and irregularities in the objective function space (*Kavetski et al.*, 2003, 2006b; *Kavetski and*

Clark., 2010; *Schoups et al.*, 2010b). These findings provide a deeper understanding of the convergence problems of local search methods, and demonstrate a need for implicit solvers that iteratively adjust the integration time step based on the state dynamics.

Research into the characterization of uncertainty has resulted in formal and informal statistical approaches. While initial attempts have focused primarily on methods to quantify parameter uncertainty (*Beven and Binley*, 1992; *Freer et al.*, 1996; *Gupta et al.*, 1998; *Kuczera and Parent*, 1998; *Vrugt et al.*, 2002, 2003a; *Wagener et al.*, 2003; *Beven*, 2006; *Vrugt and Robinson*, 2007a), emerging approaches include state-space filtering (*Vrugt et al.*, 2005; *Moradkhani et al.*, 2005a,b; *Vrugt et al.*, 2006a; *Slater and Clark*, 2006; *Reichle*, 2008; *Salamon and Feyen*, 2009; *DeChant and Moradkhani*, 2012; *Vrugt et al.*, 2012), multimodel averaging (*Butts et al.*, 2004; *Georgakakos et al.*, 2004; *Ajami et al.*, 2007; *Vrugt and Robinson*, 2007b), and various (non)Bayesian approaches to treat individual error sources and assess predictive uncertainty (*Montanari and Brath*, 2004; *Vrugt et al.*, 2005; *Kavetski*, 2006a,b; *Kuczera et al.*, 2006; *Huard and Mailhot*, 2006; *Jacquin and Shamseldin*, 2007; *Fenicia et al.*, 2007; *Marshall et al.*, 2007; *Montanari and Gross*, 2008; *Vrugt et al.*, 2008a,b; *Reichert and Mieleitner*, 2009; *Solomatine and Shrestha*, 2009; *Kuczera et al.*, 2010; *Renard et al.*, 2011). Much progress has also been made in the treatment of forcing data error (*Clark and Slater*, 2006; *Kavetski*, 2006a,b; *Vrugt et al.*, 2008a), development of a formal hierarchical framework to formulate, build and test different watershed models (*Clark et al.*, 2008), and algorithms for efficient sampling of parameter and predictive uncertainty distributions (*Kuczera and Parent*, 1998; *Vrugt et al.*, 2003a, 2008a; *Kuczera et al.*, 2010; *Laloy and Vrugt*, 2012).

Finally, research into structural adequacy has resulted in data-based mechanistic *Young* (2002, 2012), data assimilation *Vrugt et al.* (2005); *Smith et al.* (2008); *Bulygina and Gupta* (2011), and other stochastic techniques *Reichert and Mieleitner* (2009) for inference and iterative refinement of the mathematical structure of conceptual hydrologic models. This has led to the understanding that discharge data contain sufficient information to warrant the identification of a suitable model structure that mimics as closely and consistently as possible the observed watershed behavior at the temporal and spatial scale of measurement.

All this work capitalizes in some way on the "classical" error residual aggregation approach introduced in the early nineteenth century by Adrian Marie Legendre (1752 - 1833) and Carl Friedrich Gauss (1777 - 1855) for fitting simple empirical regression models to noisy data. The least squares method they proposed defines the "best" parameter values, $\boldsymbol{\theta}$ as those for which the sum of squared error, $F_{\mathrm{SLS}} = \sum_{t=1}^{n}(d_t(\boldsymbol{\theta}) - \tilde{d}_t)^2$ between the observed, $\tilde{\mathbf{D}} = \{\tilde{d}_1, \ldots, \tilde{d}_n\}$ and simulated response, $\mathbf{D}(\boldsymbol{\theta}) = \{d_1(\boldsymbol{\theta}), \ldots, d_n(\boldsymbol{\theta})\}$ is at its minimum. In 1822, Gauss was able to state that this approach is optimal if the final residual errors are uncorrelated, with zero mean, and equal variances (homoscedastic). This result is known as the Gauss-Markov theorem.

There is increasing concern surfacing in the hydrologic literature that this historical approach to model calibration introduced by Legendre and Gauss has some serious deficiencies that necessitates the development of a more powerful paradigm. One of these deficiencies is that model and forcing (input) data errors are assumed to be either "negligibly small" or to be somehow "absorbed" into the error residuals. The residuals are then expected to behave statistically similar as the calibration data measurement error. Yet, a-posteriori diagnostic checks typically demonstrate that the error residuals, $\mathbf{E}(\boldsymbol{\theta}) = \mathbf{D}(\boldsymbol{\theta}) - \tilde{\mathbf{D}} = \{e_1(\boldsymbol{\theta}, \ldots, e_n(\boldsymbol{\theta})$ exhibit considerable variation in bias, variance, and correlation structures at different parts of the model response. This is in part due to the presence of model structural and forcing (input) data errors whose contribution may, in general, be substantially larger than the (calibration) data measurement error. These errors do not necessarily have any inherent probabilistic properties that can be exploited in the construction of an explicit objective function. While we can assume an (stochastic or deterministic) error model for model structural and forcing data errors, this will be purely for the sake of mathematical convenience.

Some interesting approaches for addressing the limitations of the classical calibration approach, particularly in the context of addressing model parameter and prediction uncertainty, have begun to appear in the literature. These include the limits of acceptability approach (*Beven*, 2006; *Blazkova and Beven*, 2009), the Bayesian Total Error Analysis (BATEA) framework of Kavetski and coworkers (*Kavetski*, 2006a,b; *Kuczera et al.*, 2006; *Thyer et al.*, 2009; *Renard et al.*, 2011), the Simultaneous Optimization and Data Assimilation (SODA), DiffeRential Evolution Adaptive Metropolis (DREAM) and Particle-DREAM methodologies of Vrugt and coworkers (*Vrugt et al.*, 2005, 2012), the stochastic, time-dependent parameter approach of Reichert and coworkers (*Frey et al.,*, 2011; *Reichert and Mieleitner*, 2009), the generalized likelihood function of *Schoups and Vrugt* (2010a) combined with Markov Chain Monte Carlo (MCMC) simulation using DREAM (*Vrugt et al.*, 2008a,b, 2009a; *Laloy and Vrugt*, 2012), (Bayesian) model-averaging (*Butts et al.*, 2004; *Ajami et al.*, 2007; *Vrugt and Robinson*, 2007b), the hypothetico-inductive data-based mechanistic modeling framework of *Young* (2012) and Bayesian data assimilation (*Bulygina and Gupta*, 2011). Many of these approaches adopt a Bayesian viewpoint, and relax the assumption of a single "optimum" parameter value in favor of a posterior distribution that accurately recognizes the role of model structural, forcing data, calibration data, and parameter uncertainty (see Figure 1.1).

Figure 1.1 provides an overview of possible error sources that affect our ability to correctly describe the physical system. The error in the model output (5) originates from several sources, including (1) inadequate and/or incomplete knowledge of the model parameters, $\boldsymbol{\theta}$ (2) errors in the input (forcing) data, $\tilde{\mathbf{U}}$ and (3) initial states, $\tilde{\mathbf{x}}_0$ and (4) structural inadequacies in the model equations, and/or improper dimensionality of the state space (e.g. epistemic errors). We now like to confront the uncertain model output with the observed data $\tilde{\mathbf{D}}$ and derive estimates of each individual error source. If we adopt a Bayesian viewpoint this requires the definition of a prior distribution and likelihood function. These two functions should properly recognize the contribution of each individual error source, yet are very difficult to specify a-priori due to a lack of knowledge.

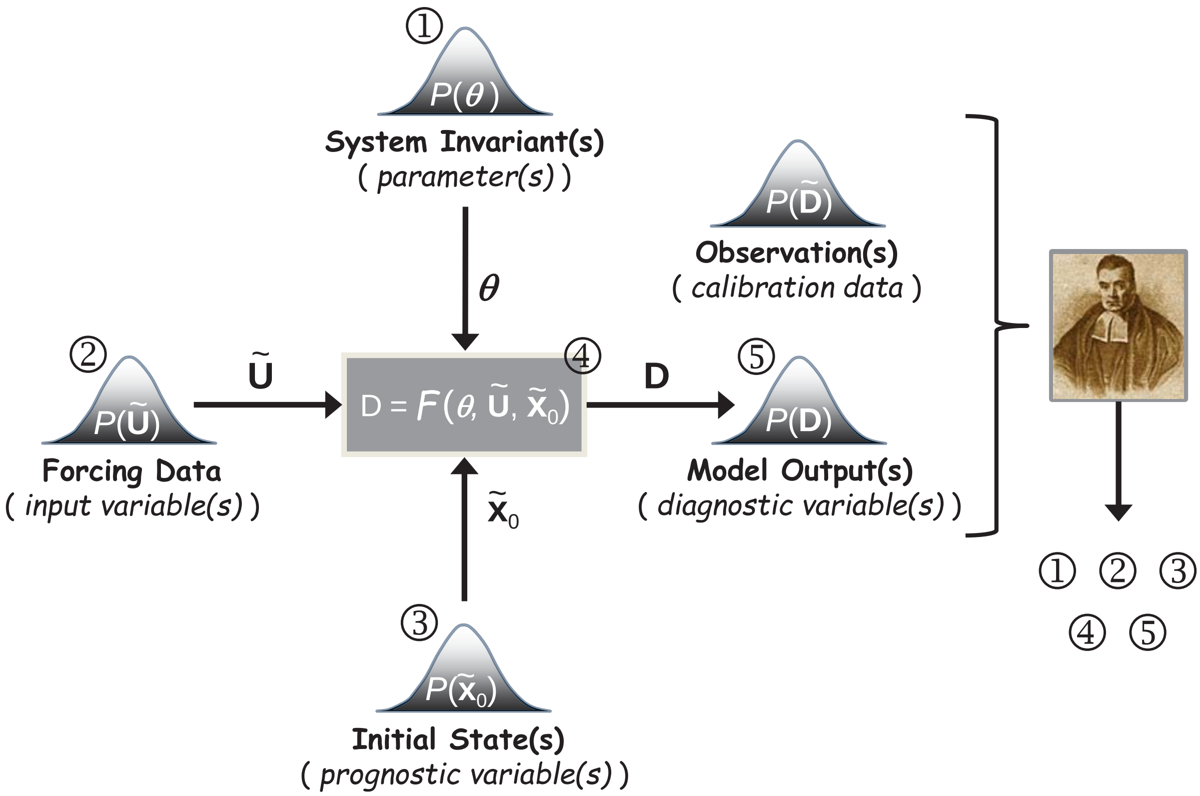

Figure 1.1: Schematic overview of the model-data fusion problem. The output simulated by the model operator (hypothesis), $\mathbf{D} = \mathcal{F}(\boldsymbol{\theta}, \tilde{\mathbf{U}}, \tilde{\mathbf{x}}_0)$ is subject to considerably uncertainty in the (1) model parameters, (2) forcing data, (3) initial states, and (4) model structure. Bayesian analysis now proceeds with inference of these error sources using the observed data, $\tilde{\mathbf{D}}$.

The need for more sophisticated approaches to model calibration and evaluation is becoming well recognized in the scientific community. For example, the Predictions in Ungaged Basins (PUB) initiative seeks to reduce predictive uncertainty through interactive learning leading to new and/or improved hydrological models (*Sivapalan et al.*, 2003); Theme 3 of the PUB initiative is titled 'Uncertainty Analysis and Model Diagnostics' (*Wagener et al.*, 2006). A broader community effort involves the move towards Environmental Observatories (EOs) in the USA and elsewhere. As stated during a recent National Science Foundation (NSF) sponsored meeting to discuss Grand Challenges of the Future for Environmental Modeling: 'Models are complex assemblies of multiple, constituent hypotheses ... that must be tested ... against the new streams of field data. Working out novel ways of conducting these tests, will be a major scientific challenge associated with the Environmental Observatories' (Beck, Presentation at NSF EO Workshop on Modeling, Tucson, AZ, April 2007). This is further expressed as Challenge 7 in the white paper resulting from the workshop:

What radically novel procedures and algorithms are needed to rectify the chronic, historical deficit (of the past four decades) in engaging complex Very High Order Models systematically and successfully with field data for the purposes of learning and discovery and, thereby, enhancing the growth of environmental knowledgethis given the expected massive expansion in the scope and volume of field observations generated by the Environmental Observatories, coupled and integrated with the prospect of equally massive expansion in data processing and scientific visualization enabled by the future environmental cyber-infrastructure? (Beck et al., 2007).

In this thesis, we will adopt a Bayesian viewpoint to model calibration and include explicit recognition of forcing data uncertainty in the calibration of rainfall-runoff models. Latent variables are used to describe rainfall data error and the resulting precipitation multipliers and model parameters are estimated using the **D**iffe**R**ential **E**volution **A**daptive **M**etropolis (DREAM) algorithm *Vrugt et al.* (2008a, 2009a). This multi-chain Markov chain Monte

Carlo (MCMC) simulation algorithm automatically tunes the scale and orientation of the proposal distribution en route to the target distribution, and exhibits excellent sampling efficiencies on complex, high-dimensional, and multi-modal target distributions. DREAM is an adaptation of the Shuffled Complex Evolution Metropolis *Vrugt et al.* (2003a) algorithm and has the advantage of maintaining detailed balance and ergodicity. Benchmark experiments *Vrugt et al.* (2008a, 2009a); *Laloy and Vrugt* (2012); *Laloy et al.* (2013); *Linde and Vrugt* (2013); *Lochbühler et al.* (2014); *Laloy et al.* (2015) have shown that DREAM is superior to other adaptive MCMC sampling approaches, and in high-dimensional search/variable spaces even provides better solutions than commonly used optimization algorithms.

Our results will elucidate a strong dependency of the posterior rainfall record on the assumed model structure used to simulate the rainfall-runoff transformation. This point was addressed in a comment of *Beven* (2008b) on *Vrugt et al.* (2009a) - and simulation results with different watershed models now explicitly demonstrate this interdependence. The inference methodology presented herein can easily be extended to include additional errors such as potential evapotranspiration or temperature. These quantities will primarily affect the streamflow response during drying conditions of the watershed. Note, the results of this thesis are of great importance for ground-verification of remote sensing data. The remainder of this thesis is organized as follows. Chapter 2 introduces the models, data, and basic building blocks of the Bayesian inference methodology used herein for rainfall error reconstruction. Section 2.1 briefly reviews Bayes law and hypothesis formulation using numerical modeling. This is followed in Section 2.2 by a detailed discussion of how to reconstruct rainfall records using latent variables (also called rainfall multipliers). In this section we are particularly concerned with the formulation of the likelihood function used for inference of the rainfall data errors. Section 2.3 then introduces the DREAM algorithm used for posterior sampling, and Section 2.4 reviews the watershed models and hydrologic data used for testing of the proposed methodology. Chapter 3 (3.1-3.3) then discusses the results of our numerical studies with the HYMOD, SAC-SMA and TOPMO conceptual watershed models. Finally, a summary with conclusions is presented in Section 3.4.

Chapter 2

Methods and data

In this Chapter we will discuss the Bayesian paradigm used for inference of the rainfall data record (hyetograph) and hydrologic model parameters. Then, we will describe a parsimonious framework for describing forcing (precipitation) data error that is similar to the methodology described by (*Vrugt et al.*, 2008a) using the DREAM algorithm. Finally, we will discuss the data and models used herein to test our methodology.

2.1 Bayes Law and numerical modeling

Bayesian methods have become increasingly popular for fitting environmental models to data. Bayes law updates the prior probability of a certain hypothesis when new data, $\tilde{\mathbf{D}} = \tilde{d}_1, ..., \tilde{d}_n$ become available. The hypothesis typically constitutes the parameter values, $\boldsymbol{\theta}$ of a model, $\mathcal{F}$ which simulates the observed data using

$$\tilde{\mathbf{D}} \leftarrow \mathcal{D}(\boldsymbol{\theta}, \tilde{\mathbf{U}}, \tilde{\mathbf{x}}_0), \tag{2.1}$$

where $\mathbf{D}$ is a vector (matrix) of output variables simulated by the model, $\mathbf{U} = \{\tilde{\mathbf{u}}_1, \ldots, \tilde{\mathbf{u}}_n\}$ is a $n \times l$ matrix of observed forcing data (e.g. daily estimates of precipitation and potential evapotranspiration; $l = 2$), $\mathbf{x} \in \mathcal{X} \in \mathbb{R}^s$ denote the s initial states, and $\boldsymbol{\theta} \in \boldsymbol{\Theta} \in \mathbb{R}^d$ signify the d model parameters.

If we now adopt Bayes theorem we can derive the posterior distribution of the parameters by conditioning the temporal behavior of the model on measurements of the observed system response. If we assume $\tilde{\mathbf{D}} = \{\tilde{d}_1, \ldots, \tilde{d}_n\}$ to be a n-vector of discharge measurements at times $t = \{1, \ldots, n\}$ which summarizes the response of some hydrologic system $\Im$ to forcing $\mathbf{U} = \{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$ then the posterior hmodel parameter distribution, $P(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}}, \mathbf{x}_0)$ can be derived from

$$P(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}}, \mathbf{x}_0) = \frac{P(\boldsymbol{\theta}, \tilde{\mathbf{U}}, \mathbf{x}_0) L(\boldsymbol{\theta}|\mathbf{D}, \tilde{\mathbf{U}}, \mathbf{x}_0)}{P(\tilde{\mathbf{D}})}, \tag{2.2}$$

where $P(\boldsymbol{\theta}, \tilde{\mathbf{U}}, \mathbf{x}_0)$ signifies the prior distribution, and $L(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}}, \mathbf{x}_0)$ denotes the likelihood function. Note that in hydrologic modeling the sensitivity of the simulator $\mathcal{F}(\cdot)$ to $\mathbf{x}_0$ diminishes with lead time. Hence, a spin-up period usually suffices to remove the dependence of the posterior distribution on $\mathbf{x}_0$.

The evidence, $P(\tilde{\mathbf{D}})$ acts as a normalization constant (scalar) so that the posterior distribution integrates to unity

$$P(\tilde{\mathbf{D}}) = \int_{\boldsymbol{\Theta}} P(\boldsymbol{\theta}, \tilde{\mathbf{U}}) L(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}}) \mathrm{d}\boldsymbol{\theta}, \tag{2.3}$$

over the parameter space. In practice, $P(\tilde{\mathbf{D}})$ is not required for posterior estimation as all statistical inferences about $P(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}})$ can be made from the product of the prior distribution and likelihood function (e.g. unnormalized density)

$$P(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}}) \propto P(\boldsymbol{\theta}, \tilde{\mathbf{U}}) L(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}}) \tag{2.4}$$

The likelihood function, $L(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}})$ summarizes, in probabilistic sense, the overall distance between the model simulation and corresponding observations. The mathematical definition of this function has been subject to considerable debate in the literature. Simple likelihood functions that assume Gaussian error residuals are statistically convenient, but this assumption is often not borne out of the probabilistic properties of the error residuals that show significant variations in bias, variance, and auto-correlation at different parts of the simulated watershed response. Such non-traditional residual distributions are often caused by forcing data and model structural errors, whose probabilistic properties are very difficult, if not impossible, to adequately characterize.

2.2 Precipitation error estimation and reconstruction

Rainfall errors propagate nonlinearly through watershed models and accumulate in the resolved state variables. Their effect is clearly visible in the simulated discharge dynamics with error residuals that deviate from a simple traditional statistical distribution, and persist well beyond the respective precipitation event. This anomaly is difficult to adequately capture in the construction of a likelihood function. Alternatively, we could use latent variables to parameterize rainfall data errors, and estimate these variables along with the model parameters. In the most extreme case we could assign each rainfall observation an independent, latent variable, but this approach is not particularly practical as the dimensionality of the parameter estimation problem would grow manifold. For instance, if a three-year record of daily discharge data is to be used for calibration purposes, a total of $2 \times 365 = 730$ latent variables would be necessary. This severely compromises the predictive capabilities of the watershed model.

A more defensible and more parsimonious implementation of this idea would use a single multiplier for each consecutive storm event. This idea was originally introduced by *Kavetski*

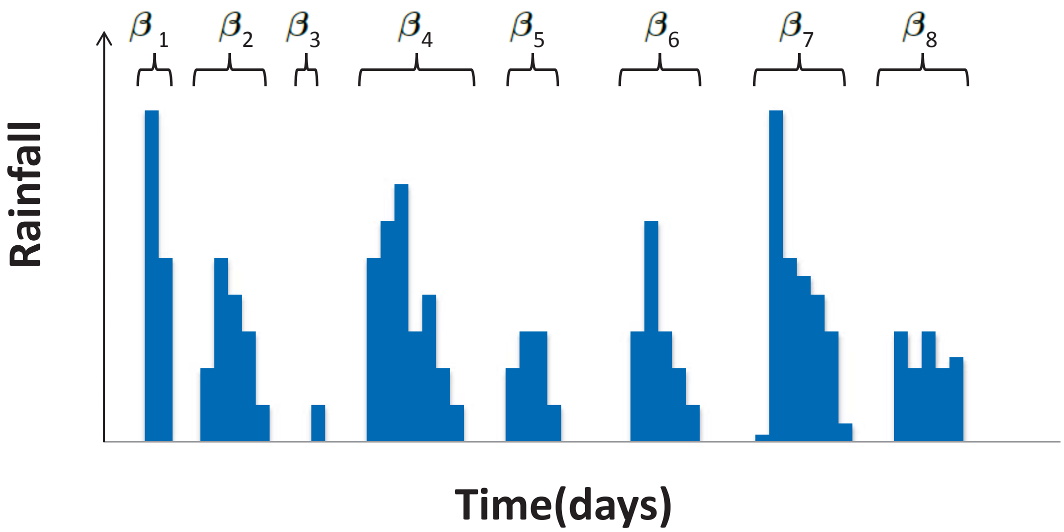

Figure 2.1: Example of how the multipliers are assigned to each storm event. These multipliers are then treated as latent variables and their posterior distribution derived along with that of the model parameters by calibration against the observed streamflow data using Bayesian inference with DREAM.

et al. (2002) and is at the heart of the BATEA methodology (*Kavetski*, 2006a,b; *Kuczera et al.*, 2006; *Renard et al.*, 2011). Prior to calibration, individual storm events are identified from the measured hyetograph and hydrograph. Each of the m storm events is assigned a different rainfall multiplier, $\boldsymbol{\beta} = \{\beta_1, \ldots, \beta_m\}$. The "true" rainfall, $\mathbf{U}$ is then assumed to follow the same pattern as the observed precipitation, $\tilde{\mathbf{U}}$ but with a simple linear error correction, $u_j = \beta_j \tilde{p}_j \; \forall j \in \{1, \ldots, m\}$ to the rainfall depths. This corrected hyetograph then serves as input to the hydrologic model. Note that this method does not correct rainfall amounts of zero, yet it provides a reasonable starting point for our analysis. The rainfall multiplier methodology is schematically explained in Figure 2.1.

2.2.1 Likelihood function used in case study A

The main culprit now resides in the definition of the likelihood function. In case A, $L(\boldsymbol{\theta}|\tilde{\mathbf{D}})$ that summarizes the overall distance between the model simulations and corresponding observations. If we assume the error residuals to be uncorrelated, Gaussian distributed with constant variance, σ_ν^2, the likelihood function can be written as

$$L(\theta|\tilde{\mathbf{D}},\tilde{\mathbf{U}}) = \prod_{t=1}^{n} \frac{1}{\sqrt{2\pi\hat{\sigma}_\nu^2}} \exp\left[-\frac{1}{2}\hat{\sigma}_\nu^{-2}(\tilde{d}_t - d_t(\boldsymbol{\theta},\tilde{\mathbf{U}}))^2\right], \tag{2.5}$$

where $\hat{\sigma}_\nu$ is an estimate of the standard deviation of the measurement error. The value of $\hat{\sigma}_\nu$ can be specified *a-priori* based on knowledge of the measurements errors, or alternatively its value can be inferred simultaneously with the values of $\boldsymbol{\theta}$ *Vrugt et al.* (2008b); *Laloy and Vrugt* (2012).

For reasons of algebraic simplicity and numerical stability, it is often convenient to consider the log-likelihood function, $\mathcal{L}(\boldsymbol{\theta}|\tilde{\mathbf{D}},\tilde{\mathbf{U}})$ rather than $L(\boldsymbol{\theta}|\tilde{\mathbf{D}},\tilde{\mathbf{U}})$ itself

$$\mathcal{L}(\boldsymbol{\theta}|\tilde{\mathbf{D}},\tilde{\mathbf{U}}) = -\frac{n}{2}\log(2\pi) - \frac{n}{2}\log(\hat{\sigma}_\nu^2) - \frac{1}{2}\hat{\sigma}_\nu^{-2}\sum_{t=1}^{n}(\tilde{d}_t - d_t(\boldsymbol{\theta},\tilde{\mathbf{U}}))^2. \tag{2.6}$$

In the absence of detailed information about the measurement error of the calibration data, it might be convenient to remove $\hat{\sigma}_\nu^2$. If we assume the variance of the error residuals to be a sufficient statistic for $\hat{\sigma}_\nu^2$ then we can derived the following simplified likelihood function

$$\mathcal{L}(\boldsymbol{\theta}|\tilde{\mathbf{D}},\tilde{\mathbf{U}}) = -\frac{n}{2}\log\left(\sum_{t=1}^{n}\left(\tilde{d}_t - d_t(\boldsymbol{\theta},\tilde{\mathbf{U}})\right)^2\right). \tag{2.7}$$

2.2.2 Likelihood function used in case study B

In case B, we use a Laplacian formulation of the likelihood function. The essential difference of this likelihood with the Gaussian formulation of case A is that a L1-norm of the residuals is used. The Laplacian likelihood function can be written as

$$L(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}}) = \prod_{t=1}^{n} \frac{1}{2\hat{\sigma}_\nu} \exp\left(-\frac{|\tilde{d}_t - d_t(\boldsymbol{\theta}, \tilde{\mathbf{U}})|}{\hat{\sigma}_\nu}\right). \tag{2.8}$$

If we assume a heteroscedastic error model, and let $\hat{\sigma}_\nu$ depend on the actual observation then this provides the following formulation of the likelihood function

$$\mathcal{L}(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}}) = -\sum_{t=1}^{n} \{\log(2\sigma_{t,\nu})\} - \sum_{t=1}^{n} \left(\frac{|\tilde{d}_t - d_t(\boldsymbol{\theta}, \tilde{\mathbf{U}})|}{\hat{\sigma}_{t,\nu}}\right) \tag{2.9}$$

2.2.3 Likelihood function used in case study C

The third and last likelihood function considered herein is taken from *Kavetski* (2006a). This likelihood function differs from those used in case A and B in that the precipitation data is considered explicitly so as to avoid the reconstructed rainfall record to deviate too much from its measured counterpart. As in *Kavetski* (2006a) it is assumed that the m multipliers $\boldsymbol{\beta}$ are described by a vague inverse gamma prior with ν degrees of freedom. The following log-likelihood function is then obtained

$$\mathcal{L}(\boldsymbol{\theta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}}) = -\frac{(m+\nu-1)}{2} \log\left\{\sum_{t=1}^{m} (\boldsymbol{\beta}_t - \mu_\beta)^2 + \nu\sigma_\beta^2\right\} - \frac{n}{2} \log\left(\sum_{t=1}^{n} \left(\tilde{d}_t - d_t(\boldsymbol{\theta}, \tilde{\mathbf{U}})\right)^2\right), \tag{2.10}$$

where μ_β and σ_β^2 denote the prior mean and variance of the rainfall multipliers. We assume that the precipitation measurements are, on average, unbiased, and hence $\mu_\beta = 1$. The variables $\{\nu, \sigma_\beta^2\}$ of the inverse gamma prior reflect the modeler's confidence in the input data. Figure 2.2 plots three different shapes of the prior distribution for different values of ν. The larger he value of ν, the degrees of freedom, the peakier the prior distribution of σ_β^2. It is apparent that this prior discourages extremely small and very large values of σ_β^2.

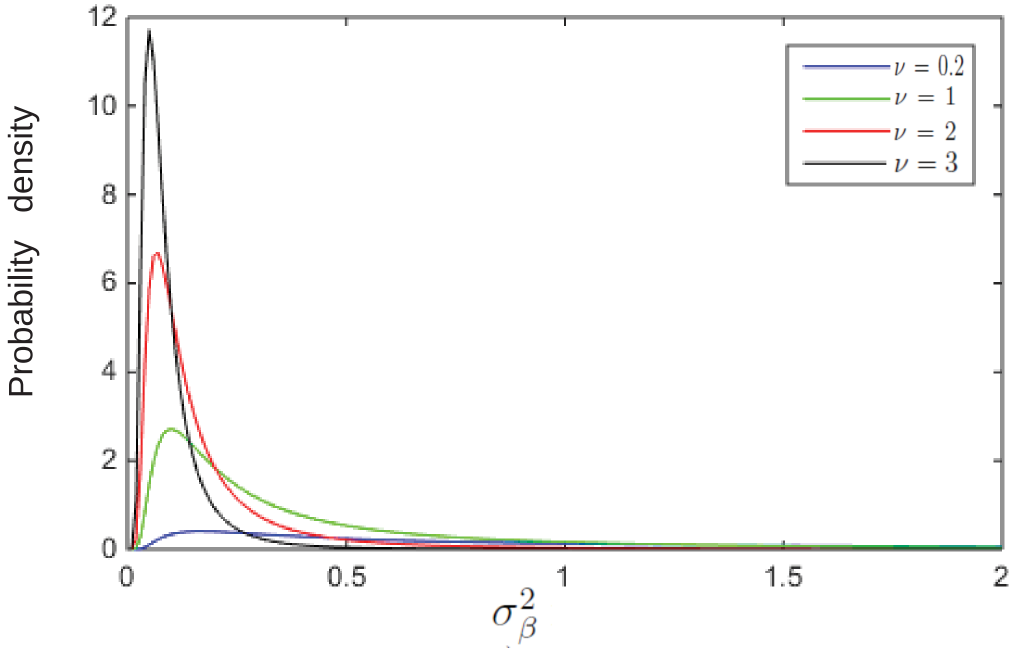

Figure 2.2: Inverse gamma prior distribution of σ_β^2 for four different degrees of freedom coded in a different color; $\nu = 0.2$ (blue), $\nu = 1$ (green), $\nu = 2$ (red), and $\nu = 3$ (black)

Kavetski (2006b) recommend setting ν so that values of σ_β^2 between 0.1 - 0.3 are somewhat favored. We use values of $\nu = 1$ and $\sigma_\beta^2 = 0.2$ in the remainder of this thesis. These values reflect an a prior expectation of likely corruption of precipitation data. A detailed derivation of Equation (2.10) appears in Appendix A - and follows *Kavetski* (2006a).

2.3 Differential Evolution Adaptive Metropolis(DREAM)

A key task in Bayesian inference is to summarize the posterior distribution. When this task cannot be carried out by analytical means nor by analytical approximation, Monte Carlo simulation methods can be used to generate a sample from the posterior distribution. The desired summary of the posterior distribution is then obtained from the sample. The posterior distribution, also referred to as the target or limiting distribution, is often high dimensional. A large number of iterative methods have been developed to generate samples from the posterior distribution. All these methods rely in some way on Monte Carlo simulation.

Vrugt et al. (2008a) introduced the Differential Evolution Adaptive Metropolis (DREAM) algorithm. This algorithm uses differential evolution as genetic algorithm for population evolution, with a Metropolis selection rule to decide whether candidate points should replace their respective parents or not. DREAM is a follow up on the DE-MC method of *ter Braak* (2006), but contains several extensions to increase search efficiency and acceptance rate for complex and multimodel response surfaces with numerous local optimal solutions. Such surfaces are frequently encountered in hydrologic modeling. The DREAM algorithm has it roots within DE-MC but uses subspace sampling and outlier chain correction to speed up convergence to the target distribution. Subspace sampling is implemented in DREAM by only updating randomly selected dimensions of $\boldsymbol{\theta}_{t-1}^{i}$ each time a proposal is generated. If A is a subset of D-dimensions of the original parameter space, $\mathbb{R}^D \subseteq \mathbb{R}^d$, then a jump in the ith chain, $i = \{1, \ldots, N\}$ at iteration $t = \{2, \ldots, T\}$ is calculated using different evolution *Storn and Price* (1997); *Price et al.* (2005)

$$\begin{aligned} \mathrm{d}\boldsymbol{\theta}^{i,A} &= (\mathbf{1}_D + \boldsymbol{\lambda}_D)\gamma_{(\delta,D)} \sum_{j=1}^{\delta} \left(\boldsymbol{\theta}_{t-1}^{\mathbf{r}_j^1,A} - \boldsymbol{\theta}_{t-1}^{\mathbf{r}_j^2,A} \right) + \boldsymbol{\zeta}_D \\ \mathrm{d}\boldsymbol{\theta}^{i,\neq A} &= 0, \end{aligned} \tag{2.11}$$

where $\gamma = 2.38/\sqrt{2\delta D}$ is the jump rate, δ denotes the number of chain pairs used to generate the jump (default is 3), and $\mathbf{r}^1$ and $\mathbf{r}^2$ are vectors consisting of δ integer values drawn without replacement from $\{1, \ldots, i-1, i+1, \ldots, N\}$.

The values of $\boldsymbol{\lambda}$ and $\boldsymbol{\zeta}$ are sampled independently from $\mathcal{U}_D(-c, c)$ and $\mathcal{N}_D(0, c^*)$ with, typically, $c = 0.1$ and c^* small compared to the width of the target distribution, $c^* = 10^{-12}$ say. With a probability of 20% we set the jump rate to 1, or $p_{(\gamma=1)} = 0.2$ to enable jumping between disconnected posterior modes. The candidate point of chain i at iteration t then becomes

$$\boldsymbol{\theta}_p^i = \boldsymbol{\theta}_{t-1}^i + \mathrm{d}\boldsymbol{\theta}^i, \tag{2.12}$$

and the Metropolis ratio is used to determine whether to accept this proposal or not.

In DREAM a geometric series of n_{cr} different crossover values is used, $\mathrm{CR} = \{\frac{1}{n_{\mathrm{cr}}}, \frac{2}{n_{\mathrm{cr}}}, \ldots, 1\}$. The selection probability of each crossover value is assumed equal at the start of simulation and defines a vector $\mathbf{p}_{\mathrm{cr}}$ with n_{cr} copies of $\frac{1}{n_{\mathrm{cr}}}$. For each different proposal the crossover, cr is sampled randomly from a discrete multinomial distribution, $\mathrm{cr} = \mathcal{F}(\mathrm{CR}, 1, \mathbf{p}_{\mathrm{cr}})$. Then, a vector $\mathbf{z} = \{z_1, \ldots, z_d\}$ with d standard uniform random labels is drawn from a standard multivariate uniform distribution, $\mathbf{z} \sim \mathcal{U}_d(0, 1)$. All those dimensions j for which $z_j \leq \mathrm{cr}$ are stored in A and span the subspace that will be sampled. In the case that A is empty, one dimension of $\boldsymbol{\theta}_{t-1}$ will be sampled at random.

The number of dimensions stored in A ranges between 1 and d and depends on the actual crossover value used. This randomized strategy, activated when $\mathrm{cr} < 1$, constantly introduces new directions that chains can take outside the subspace spanned by their current positions. This relatively simple randomized selection strategy enables single-site Metropolis sampling (one dimension at a time), Metropolis-within-Gibbs (one or a group of dimensions) and regular Metropolis sampling (all dimensions). In principle, this allows using $N < d$ in DREAM, an important advantage over DE-MC that requires $N = 2d$ chains to be run in parallel *ter Braak* (2006).

2.4 Models and data

To illustrate the rainfall estimation method discussed herein, we use historical data from the Leaf River watershed in the USA. The data consists of mean daily precipitation (mm/d),

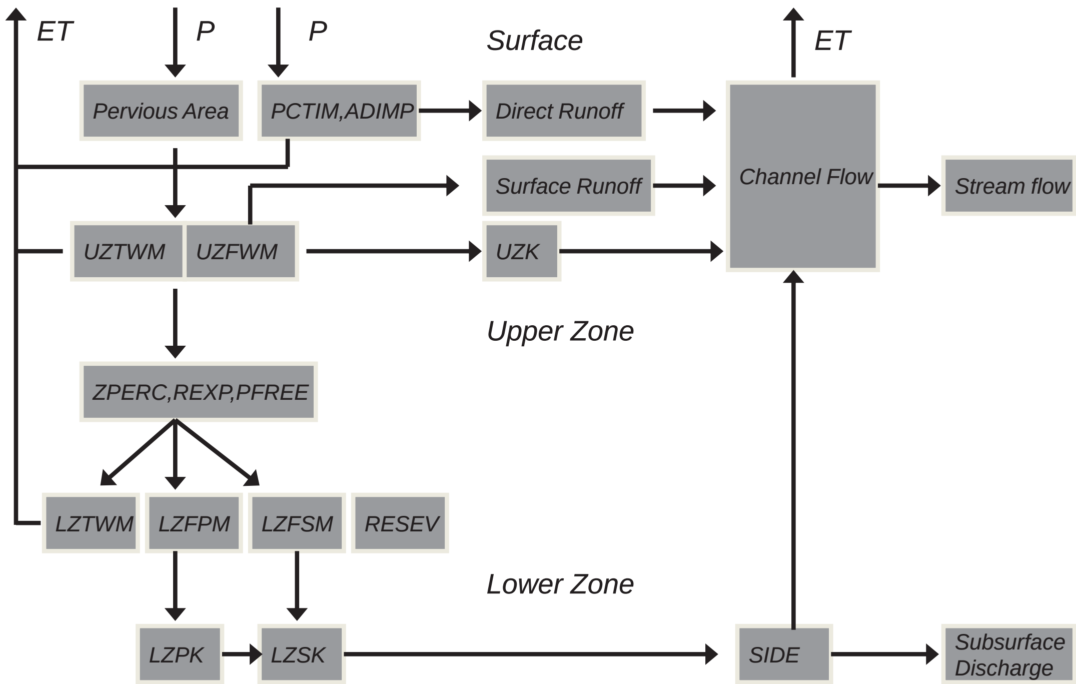

Figure 2.3: Schematic overview of the SAC-SMA watershed model

potential evapotranspiration (mm/d), and streamflow (m^3/s). A two-year record of streamflow data is used for inference of the rainfall multipliers and model parameters. In this 2 year calibration time series, a total of $m = 126$ storm events were identified.

We consider the Sacramento soil moisture accounting (SAC-SMA) model introduced by *Burnash et al.* (1973) in the early 1970s and used by the US National Weather Service (NWS) for flood forecasting throughout the United States. The model is one of the components of the NWSRFS used to convert precipitation input into streamflow outputs. A schematic overview of the SAC-SMA model is given in Figure 2.3. The parameters of the SAC-SMA model are listed in Table 2.1 along with their prior uncertainty ranges.

The second model used in our analysis involves the five-parameter Hydrologic Model, also referred to in the literature as HYMOD. This model, developed by *Boyle* (2000), consists of a relatively simple rainfall excess model, described in detail by *Moore* (1985), connected with two series of linear reservoirs (three identical quick reservoirs, and a single reservoir for

Table 2.1: Prior ranges of the SAC-SMA model parameters

Parameter	Description	Ranges
UZTWM	Upper zone tension water maximum storage	1-150
UZFWM	Upper zone free water maximum storage	1-150
UZK	Upper zone free water lateral depletion rate	0.1-0.5
PCTIM	Impervious fraction of watershed area	0-0.1
ADIMP	Additional impervious area	0-0.4
ZPERC	Maximum percolation rate	1-250
REXP	Exponent of percolation rate	1-5
LZTWM	Lower zone tension water maximum storage	1-500
LZFSM	Lower zone free water maximum supplemental storage	1-1000
LZFPM	Lower zone free water maximum primary storage	1-1000
LZSK	Lower zone supplemental free water depletion rate	0.01-0.25
LZPK	Lower zone primary free water depletion rate	0.0001-0.025
PFREE	Fraction of percolating from upper to lower zone free water storage	0-0.6

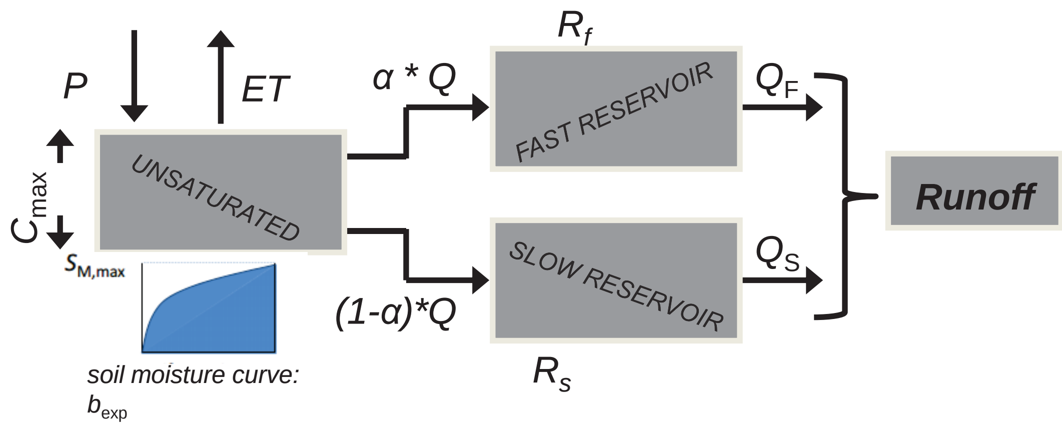

Figure 2.4: Schematic representation of the HYMOD conceptual rainfall-runoff model

Table 2.2: Prior ranges of the HYMOD model parameters

Parameter	Description	Ranges
$C_{\max}$	Maximum storage in watershed	1-500
$b_{\exp}$	Spatial variability of soil moisture storage	0.1-2.0
$Alpha$	Distribution factor between two reservoirs	0.1-0.99
R_s	Residence time slow flow reservoir	0-0.1
R_q	Residence time quick flow reservoir	0.1-0.99

the slow response). Figure 2.4 present a schematic description of HYMOD. The parameters this model are listed in Table 2.2.

As third model we use the TOPMO model *Oudin et al* (2005). This eight-parameter hydrologic model is derived from TOPMODEL *Beven* (1979). The model is schematically depicted in Figure 2.5 and the parameters and their prior uncertainty ranges are summarized in Table 2.3.

For each of the model parameters we assume a uniform (flat) prior distribution using the ranges listed in each of the Tables.

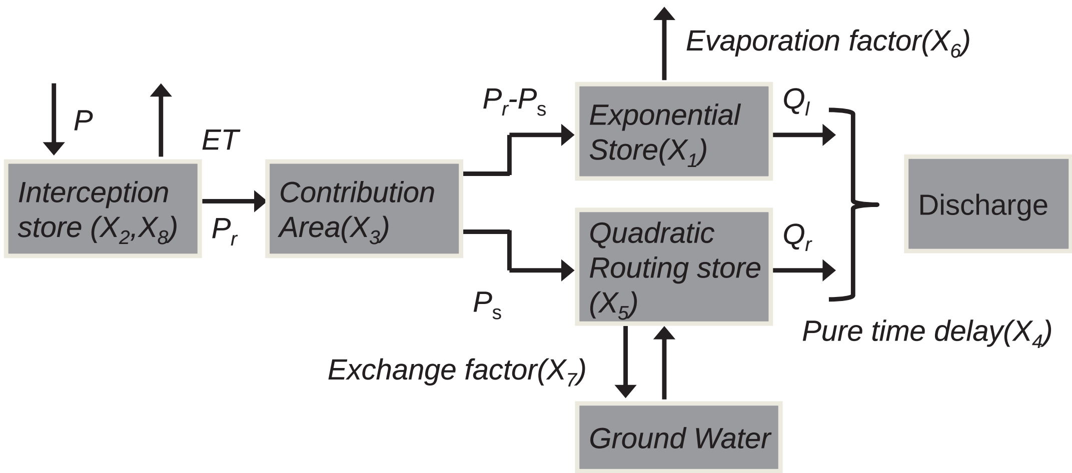

Figure 2.5: Schematic overview of the TOPMO watershed model

Table 2.3: Prior ranges of the TOPMO model parameters

Parameter	Description	Ranges
X_1	Recession coefficient of the exponential store	0-10
X_2	Capacity of the interception store	0-10
X_3	Topography index parameter	0-10
X_4	Time delay	0-1
X_5	Capacity of the routing store	0-10
X_6	Evaporation parameter	0-10
X_7	Groundwater exchange coefficient	0-10
X_8	Capacity of the production store	0-10

Chapter 3

Result and discussion

3.1 Case study A

In this case study, we fit the precipitation data using only discharge data. The likelihood function is Gaussian described as Equation 2.7. Here we use the 3 different models introduced above(HYMOD, TOPMO and SAC-SMA) to calibrate by 2 years precipitation data for Leaf River.

Figure 3.1 is created by calibration using DREAM with population N=5 chains and a generation number of 50,000. This figure presents the 95 percent streamflow uncertainty range for the selected period for Leaf River basin. With the red dot representing the observed discharge data and the RMSE Table 3.1, they indicate that we obtain a good match in all three models. This is because we adjusted the rainfall multipliers to runoff and the value of multipliers can vary to get the best fit. As a result, the boxplot of each multiplier in Figure 3.2 shows that the multipliers have a relatively large uncertainty range. Furthermore, we can find that the mean values of many multiplier distributions indicate that we have adjusted the original rainfall data too much. The multipliers cannot be larger or smaller than one too

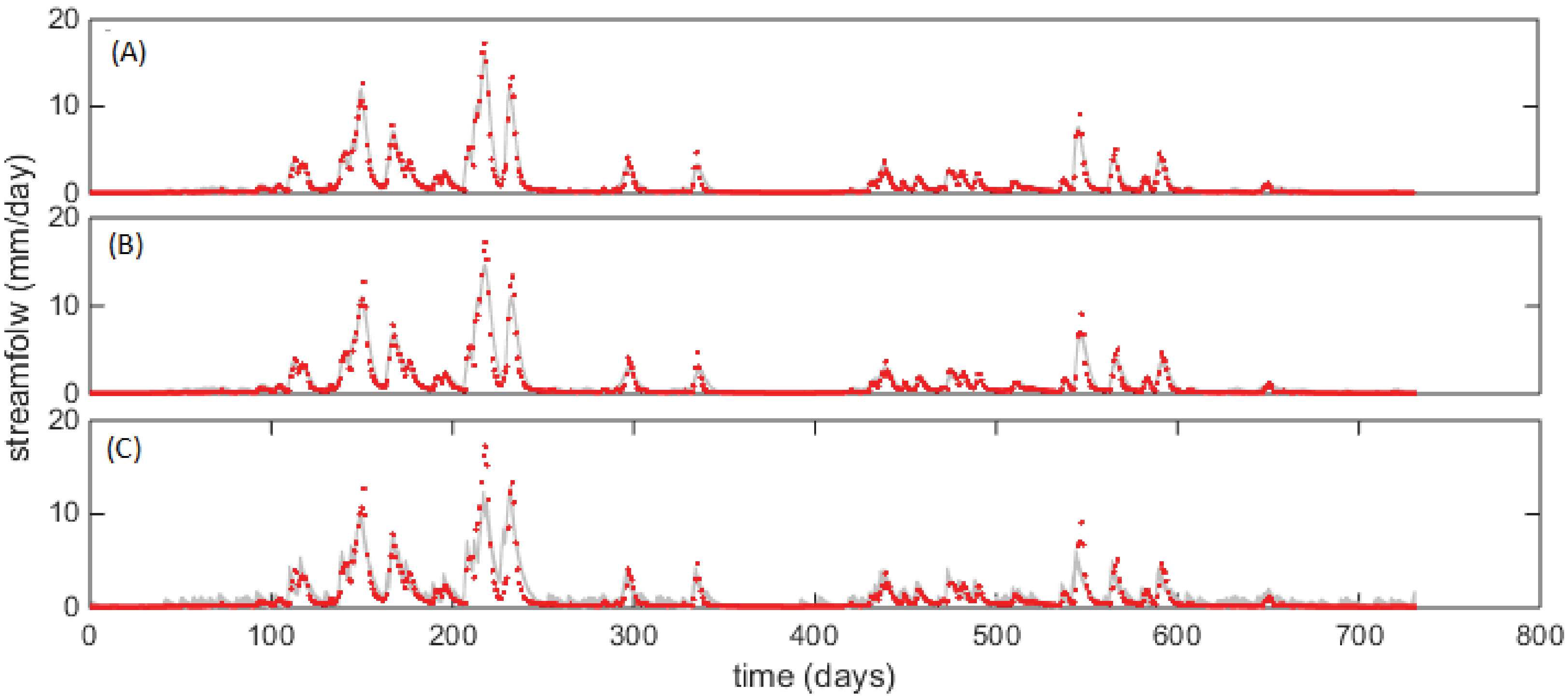

Figure 3.1: Gaussian likelihood function: 95% streamflow simulation uncertainty ranges of the HYMOD (A: top), SAC-SMA (B: middle) and TOPMO (C: bottom) conceptual watershed models. The observed data are indicated with the dots

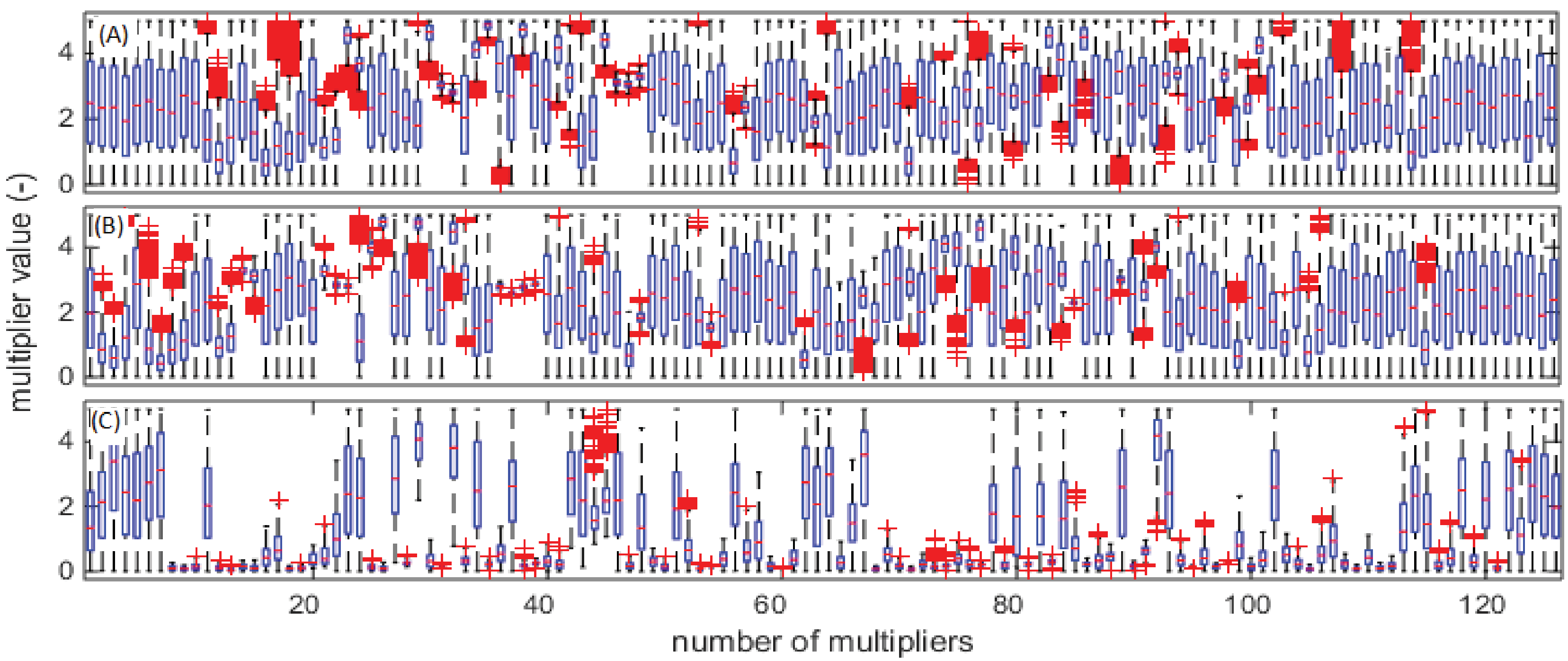

Figure 3.2: Gaussian likelihood function: Boxplot figure of the posterior rainfall multipliers derived from Bayesian analysis using DREAM. The different panels pertain to the HYMOD (A: top), SAC-SMA (B: middle) and TOPMO (C: bottom) conceptual watershed models

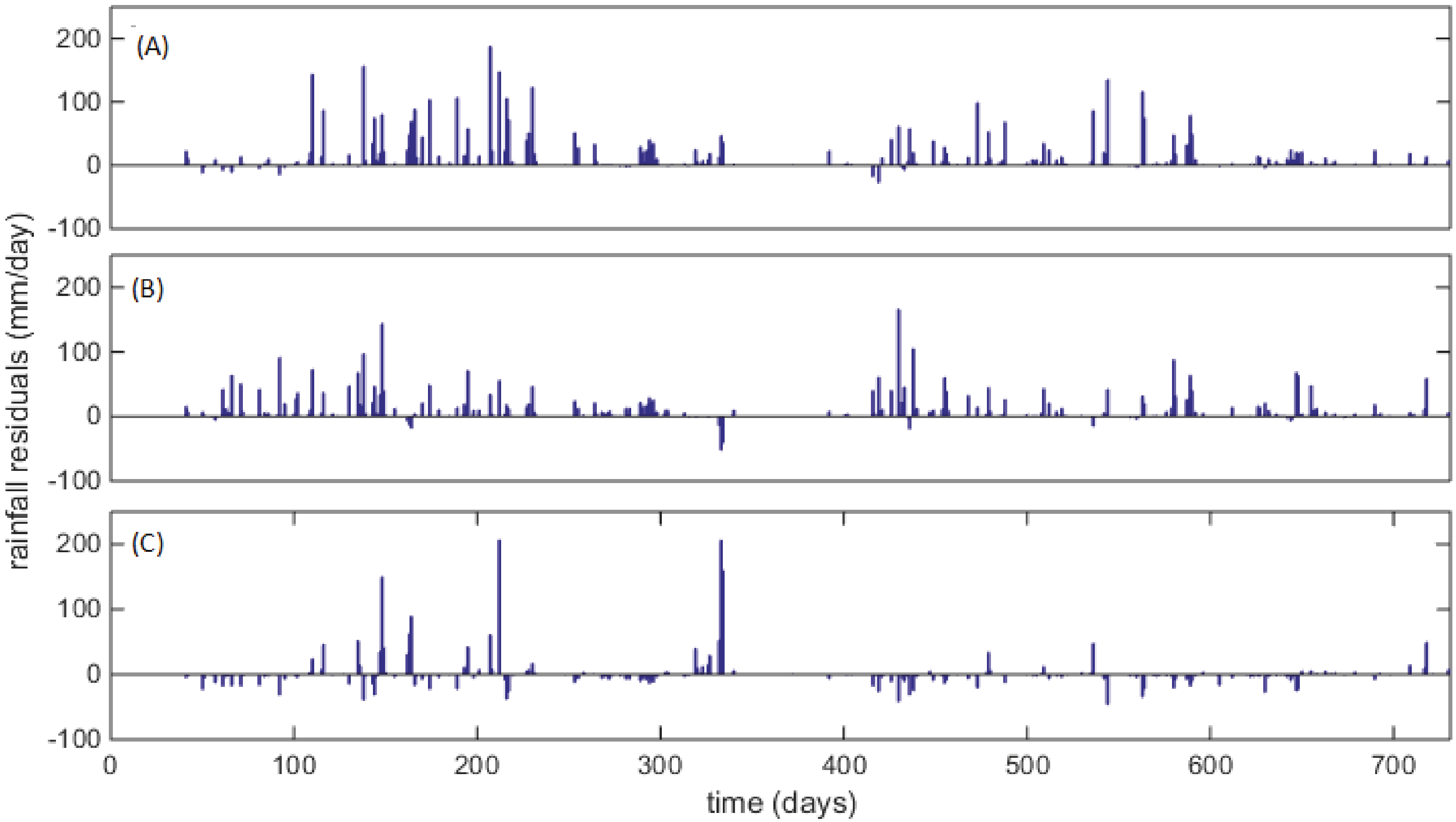

Figure 3.3: Gaussian likelihood function: Residuals figure of the reconstructed rainfall with original rainfall. The different panels pertain to the HYMOD (A: top), SAC-SMA (B: middle) and TOPMO (C: bottom) conceptual watershed models

Table 3.1: RMSE of HYMOD, SAC-SMA and TOPMO conceptual watershed models in Case study A

Model	RMSE(mm/day)
HYMOD	0.522
TOPMO	0.970
SACSMA	0.568

much based on physical meaning. The deviation between multipliers and the original rainfall data is shown in the Figure 3.3, which plots the residuals between reconstructed rainfall data and original rainfall data.

HYMOD simulation results with a 95 percent uncertainty range are shown in the top panel of Figure 3.1. Most of the peak streams are clearly identified by the simulation, and the mismatch between observation and simulation is relatively small in the figure. But when it comes to the multipliers distribution, we find that many multipliers have a relatively large uncertainty range in Figure 3.2 compared to the other case study. Several multipliers have relatively large mean values like $\beta = 23, 47.....$ The mean value > 4 indicate we have adjusted the original rainfall data by increasing 3 times. Such a value is unrealistic in the natural environment since the measurement error cannot be so large. The problem is further discussed in case study C. Similar to HYMOD, SAC-SMA model suffers almost the same issue. $\beta = 25, 26, 29....$ at the middle panel of Figure 3.2 also have a large, unrealistic mean value. But the multipliers optimized by the SAC-SMA model are different from the multipliers optimized by HYMOD. The bottom panel is the TOPMO model simulation results, which are not as good as those in the other two. We can identify some mismatches in Figure 3.1. As they are distinct from from HYMOD and SAC-SMA model, the multiplier distributions of the TOPMO model have very small mean value, which indicates no storm events. This is also unrealistic even if we consider the measurement error. This inconsistency of the boxplot results of these three models indicate that the optimized rainfall records have a significant dependence on model structure.

3.2 Case study B

In this case study, we fit the precipitation data by also only considering discharge, but we use the Laplace likelihood function. This means we use the sum of absolute residuals instead of the sum of squared residuals, as introduced in equation 2.9. The data, models and settings of DREAM are same the as in case study A.

As Figure 3.4 and Table 3.2 shows, the simulation results are also good fit with the runoff data, but this is not the case for SAC-SMA model. Another finding is that the uncertainty range for each rainfall multiplier is narrow, which demonstrates that the multipliers are more well-defined, as shown in Figure 3.5. This method encounters the same problem as case A. The deviation between multipliers and the original rainfall data is shown in the Figure 3.6, which plots the residuals between reconstructed rainfall data and original rainfall data. This study also indicates that we need to consider the deviation between multipliers and the original rainfall data in the likelihood function. Still, there is variance in the multipliers created by three models.

Compared with Case study A, Laplace - the L1 norm of sum of absolute residuals- indicates the larger residual will not dominate the likelihood, as we do not square the residuals. Therefore, it will make residuals take on the same effect as in the optimization. As shown in the simulation results presented in Figure 3.4, the HYMOD and TOPMO model all perform well. There is no significant mismatch discovered in the top and bottom panel, but the SAC-SMA model in the middle panel misses many peak streams in the observation. When it comes to the boxplot of the multiplier distributions of each model(see Figure 3.5), in contrast to Case A, the uncertainty range are very small. The better definition of multipliers in this

Table 3.2: RMSE of HYMOD, SAC-SMA and TOPMO conceptual watershed models in Case study B

Model	RMSE(mm/day)
HYMOD	0.656
TOPMO	0.722
SACSMA	0.842

figure shows that the L1 norm has an advantage over L2 norm because of its well-defined parameter values.

Although the multipliers are well-defined, the inconsistency of the boxplot results for those three models occurs similarly to case A. The fit of each model is presented by its multipliers, and these multipliers vary significantly. We can easily observed this phenomenon in Figure 3.5. When $\beta = 3$, the HYMOD at the top panel shows has a multplier distribution mean value larger than 4, but the SAC-SMA and TOPMO model indicate that the same multiplier $\beta = 3$ has an mean value less than 1. This is an obvious example of the contrast between models. The same conclusion that we can obtain from case A is that the optimized rainfall records have a significant dependence on model structure itself. The complexity, assumptions in the models, hydrology basis of each model make optimized rainfall record relatively sensitive.

Also the same issue as case A, Many multipliers distribution have a relatively large or small mean value compared with 1, that is the original rainfall data, for instance $\beta = 26, 27$ of the HYMOD model at top panel in Figure 3.5, $\beta = 30, 45$ of the SAC-SMA model at middle panel and $\beta = 23, 63, 66, 67$ of the TOPMO model at bottom panel. These all reflect to the error in assumption of likelihood function that the multipliers can vary freely to get the best fit of runoff observation.

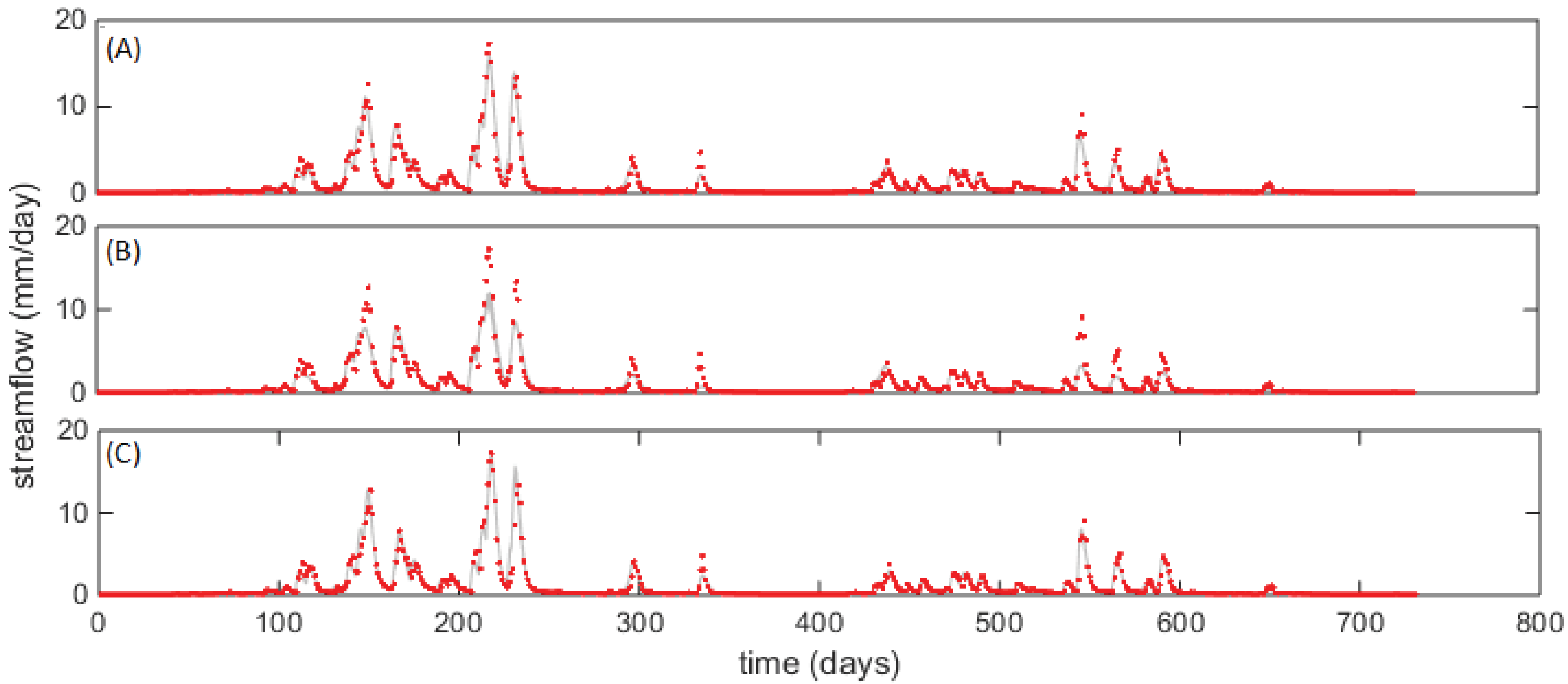

Figure 3.4: Laplacian likelihood function: 95% streamflow simulation uncertainty ranges of the HYMOD (A: top), SAC-SMA (B: middle) and TOPMO (C: bottom) conceptual watershed models. The observed data are indicated with the dots

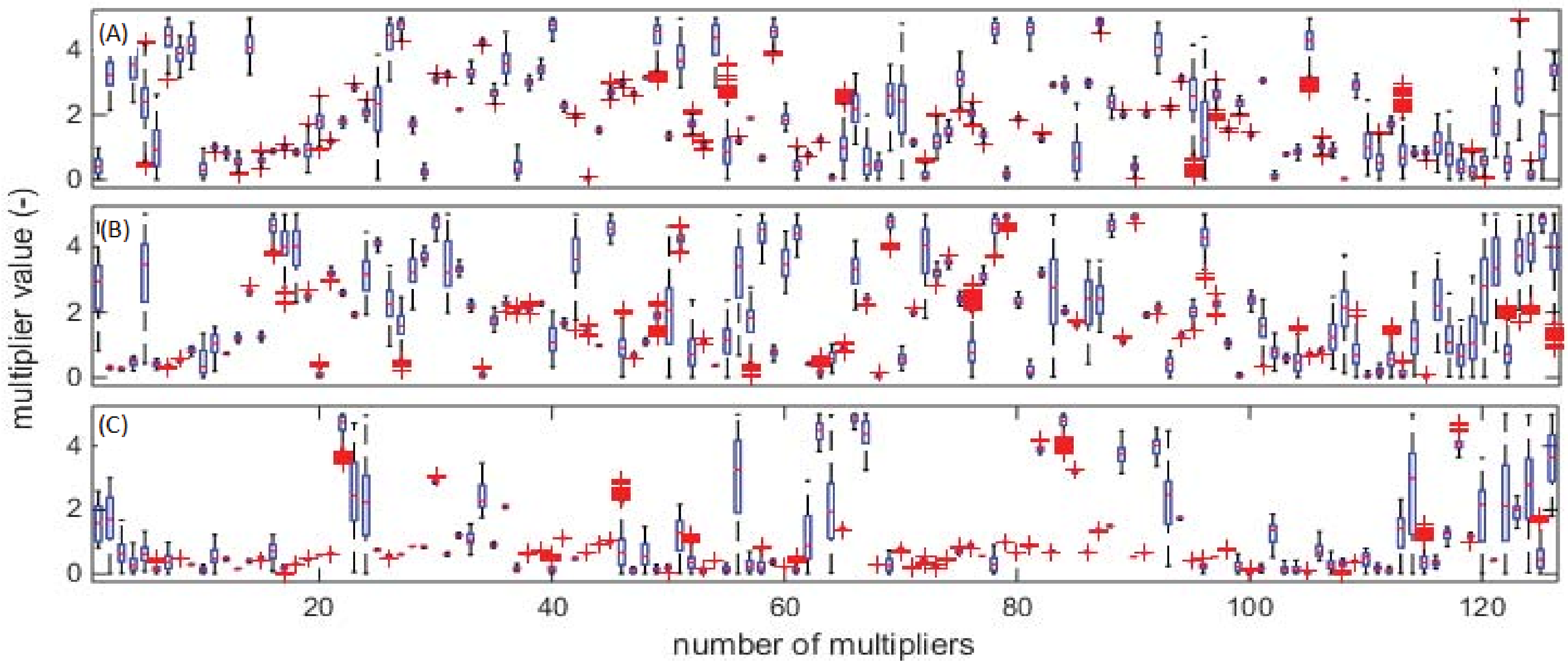

Figure 3.5: Laplacian likelihood function: Boxplot figure of the posterior rainfall multipliers derived from Bayesian analysis using DREAM. The different panels pertain to the HYMOD (A: top), SAC-SMA (B: middle) and TOPMO (C: bottom) conceptual watershed models

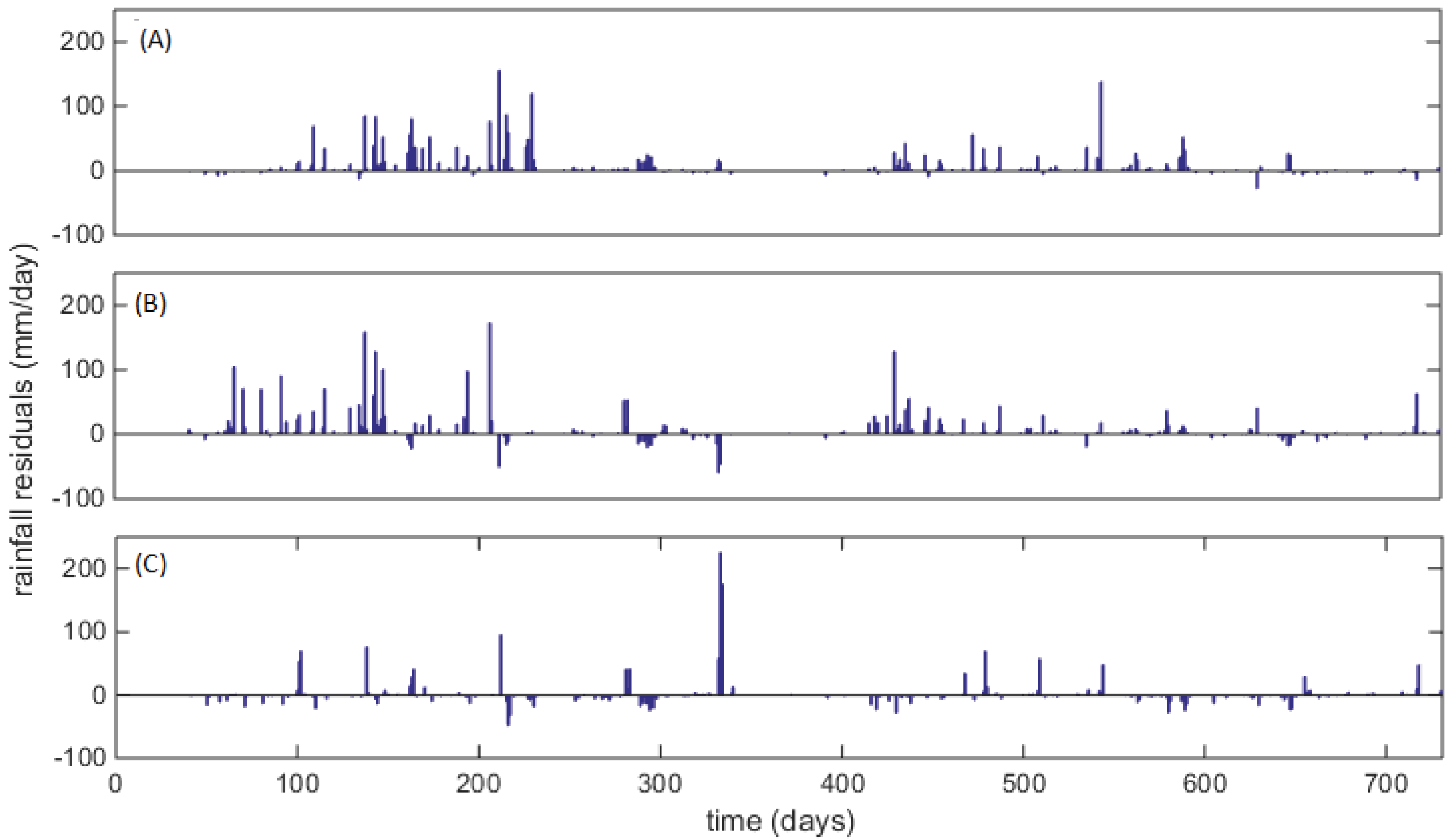

Figure 3.6: Laplacian likelihood function: Residuals figure of the reconstructed rainfall with original rainfall. The different panels pertain to the HYMOD (A: top), SAC-SMA (B: middle) and TOPMO (C: bottom) conceptual watershed models

3.3 Case study C

In this case study, we not only fit the precipitation data using the discharge but also using the original rainfall data as the likelihood function shown in equation 2.10. This method can avoid reconstructed rainfall deviated too much from measured data by adding an optimization part in the likelihood function to evaluate the distances between original and reconstructed rainfall records, which are shown in Figure 3.9.

The 95 percent streamflow uncertainty range for the selected period in Figure 3.7 and the RMSE Table 3.3 shows that we still have a good fit on observation data even if we include the evaluation part of distance between original and reconstructed rainfall for both 3 models. We can clear identify that the multipliers distributions mean are all around one in Figure 3.8. These results shows that the reconstructed rainfall data are not deviated too much from the original precipitation data. Also, the multipliers distributions are not too wide in the figure because of well-defined multipliers, and the multipliers of three models is relatively similar to each other. This similarity is because we include original rainfall data in the likelihood function. This similarity does not means that the model structure has no influence on the optimized rainfall data since there are still some differences between the multipliers with these models(but not so obvious compared with case A and B).

The accurate simulation in Figure 3.7 show that the Kavetski approach *Kavetski* (2006a) do not ruin best fit towards observation data. The evaluation part of residuals between original and reconstructed rainfall does not inflect the accuracy of simulation. The HYMOD at top panel, SAC-SMA model at middle panel and TOPMO model at bottom panel in Figure 3.7 all have a relatively high quality simulation, as there is no obvious mismatch or wrong prediction occur. However, the boxplot results not only have a fully well-defined multipliers as the narrow distribution shown in the figure, but also control the mean value of multiplier distribution around 1. It is very meaningful study through the optimized multipliers so that

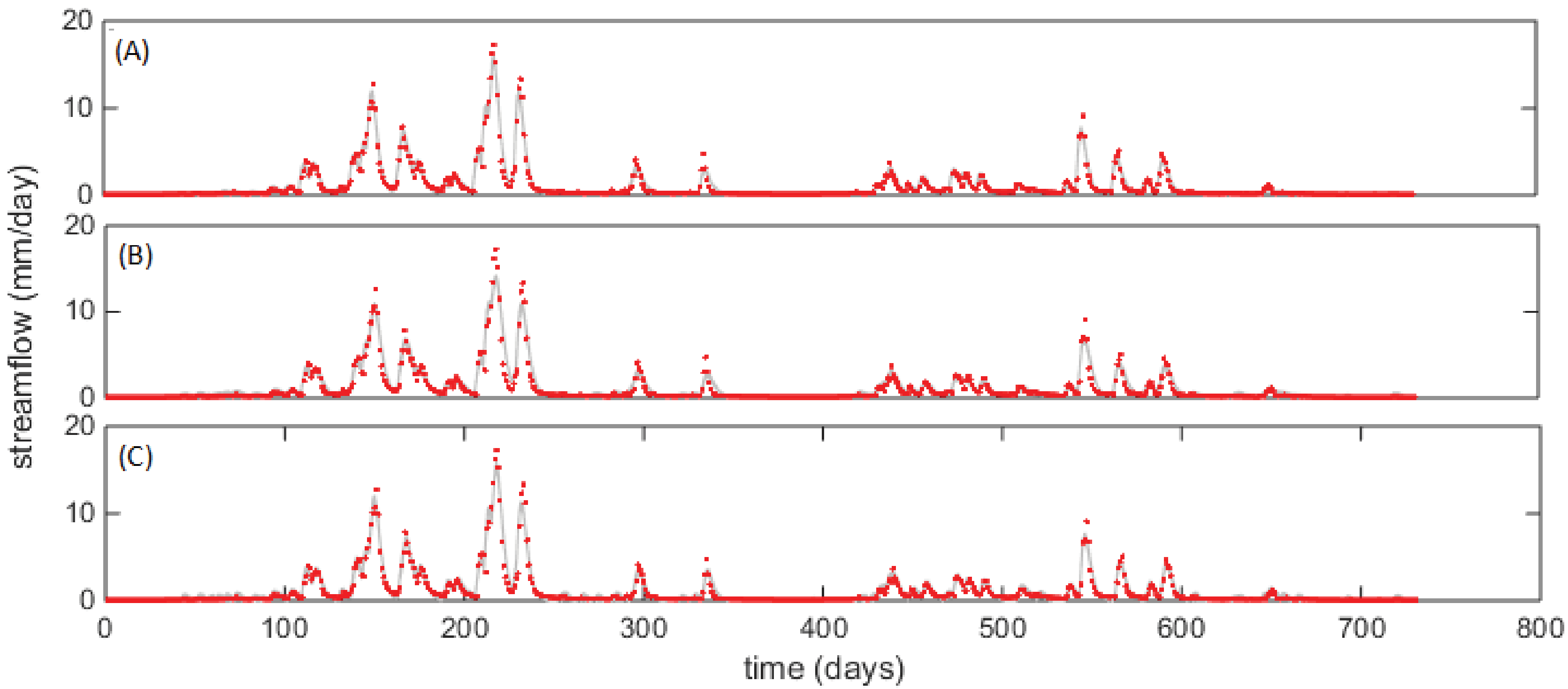

Figure 3.7: Joint likelihood function: 95% streamflow simulation uncertainty ranges of the HYMOD (A: top), SAC-SMA (B: middle) and TOPMO (C: bottom) conceptual watershed models. The observed data are indicated with the dots

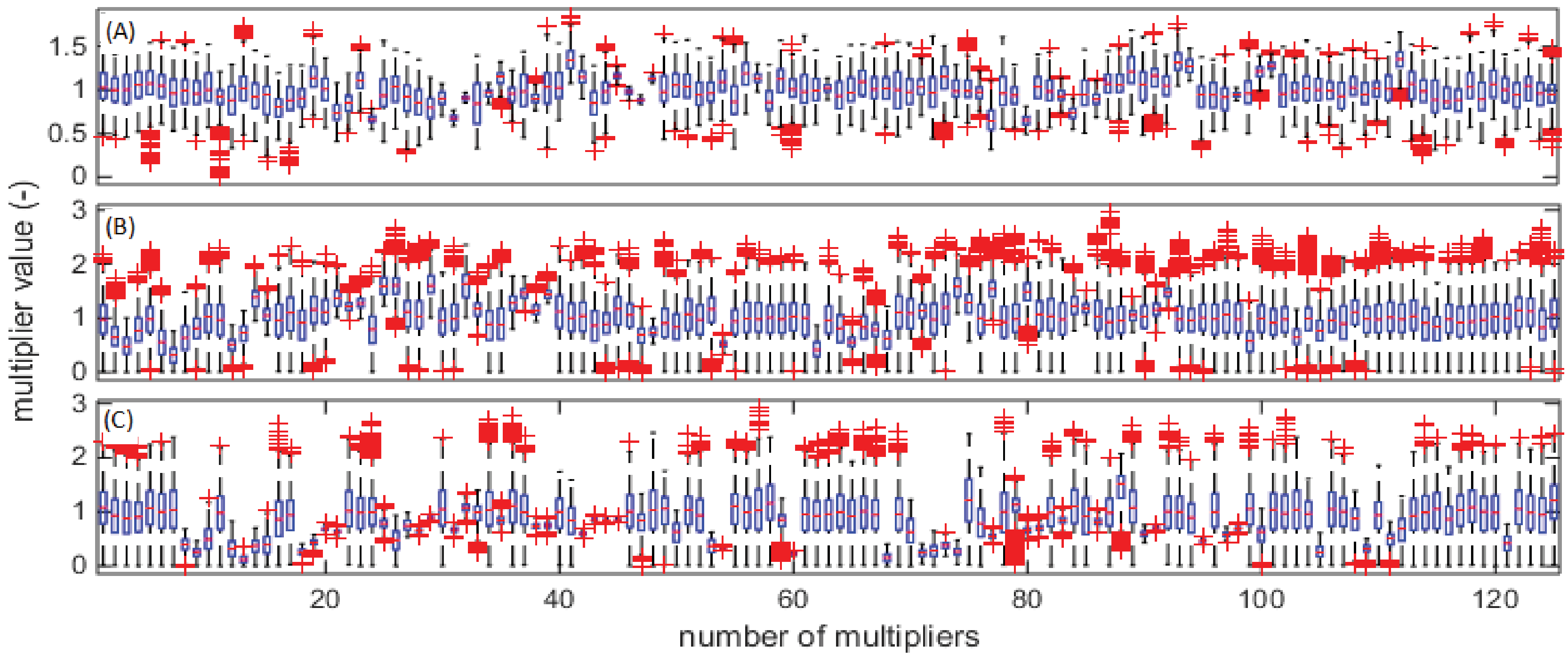

Figure 3.8: Joint likelihood function: Boxplot figure of the posterior rainfall multipliers derived from Bayesian analysis using DREAM. The different panels pertain to the HYMOD (A: top), SAC-SMA (B: middle) and TOPMO (C: bottom) conceptual watershed models

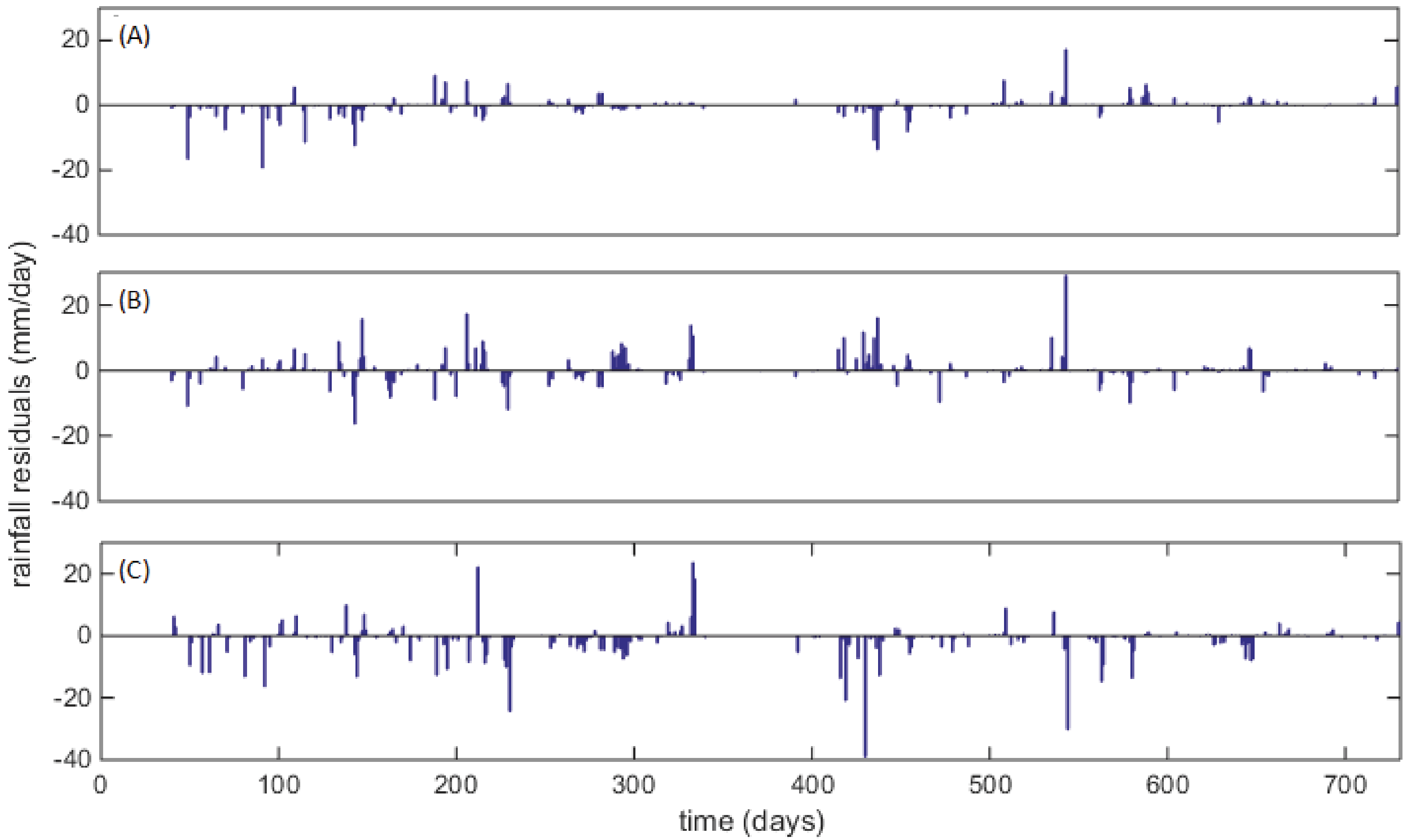

Figure 3.9: Joint likelihood function: Residuals figure of the reconstructed rainfall with original rainfall. The different panels pertain to the HYMOD (A: top), SAC-SMA (B: middle) and TOPMO (C: bottom) conceptual watershed models

Table 3.3: RMSE of HYMOD, SAC-SMA and TOPMO conceptual watershed models in Case study C

Model	RMSE(mm/day)
HYMOD	0.516
TOPMO	0.532
SACSMA	0.588

we can have a exact reflection of measurement error contained in our calibration. After we carefully observe TOPMO model at the bottom panel in Figure 3.8, there are some multipliers very close to 0 like $\beta = 13, 18$. These zero multipliers value indicate no rain or no storm event in this period of time. But these values do not exist in HYMOD and SAC-SMA model simulation, for example the $\beta = 13, 18$ I mentioned above. This variance between models reflect the conception that the optimized rainfall record significantly depend on model structure itself again.

3.4 Conclusion

Different from most publications in the literature, we have analyzed herein the influence of precipitation data errors on the posterior model parameter distributions and the simulated streamflow data. The framework used herein is based on the Bayesian paradigm and the DREAM algorithm was used to derive the posterior distribution of the hydrologic model parameters and rainfall multipliers used to characterize precipitation data uncertainty. The DREAM toolbox supports parallel computing and includes tools for convergence analysis of the sampled chain trajectories and post-processing of the results. The most important results for the Leaf River watershed and HYMOD, SAC-SMA and TOPMO conceptual watershed models are as follows

1 Joint estimation of the rainfall record and model parameters significantly enhances the quality of fit to the observed streamflow data.

2 The posterior rainfall record depends strongly on the assumed model structure used to simulate the rainfall-runoff transformation. The rainfall multipliers of the HYMOD, SAC-SMA and TOPMO model differ substantially - and exhibit a quite different temporal pattern. The posterior rainfall record thus compensates in part for structural (epistemic) errors in the model used to describe the rainfall-runoff transformation of the Leaf River watershed.

3 The posterior rainfall record and model parameter distributions depend strongly on the assumed likelihood function. The worst results are obtained if a Laplacian likelihood function is used involving a L1-norm of the error residuals.

4 The best results are obtained if precipitation and streamflow data are jointly considered in the likelihood function. This does require an informative prior distribution of the standard deviation of the rainfall multipliers - otherwise the posterior distribution is unbounded.

Subsequent work has to validate the retrieved rainfall records against precipitation estimates from remote sensing data. This will shed light on which of the three different models is most appropriate hydrologically - indeed that watershed model that provides a rainfall record which is closest to the observed data exhibits the "best" structure.

Several improvements can be made to the approach presented herein. First of all, multiple models should be considered simultaneously in our analysis to make sure that the rainfall record does not compensate for the weaknesses of a single watershed model. Second, the methodology should be applied to a much longer streamflow data set. A two year is insufficient to draw generalized conclusions - although we posit that the conclusions of this thesis will hold for those longer records as well. Third, more emphasis is required on the posterior parameter distributions - those have not been assessed in detail in the present thesis - but will be the focus on additional research. The rainfall record that is derived using the multimodel approach should be validated against other rainfall products. The premise of this methodology is that it can act as ground truth for calibration of remote sensing radar retrievals. This would improve the reliability of remote sensing precipitation data products. Note, that a better strategy is warranted to correct the observed rainfall record - the multiplier approach works in practice, but becomes cumbersome if a long streamflow data record is used with a large number of storm events. Also, days with zero rainfall are not corrected in the present analysis - which is quite a limitation as one some of these days the hydrograph is increasing - indicating a nonzero precipitation day.

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Appendix

A

If we assume the m storm depths of the rainfall record to be corrupted with some multiplicative Gaussian distribution with mean μ_β and (known) variance, σ_β^2 the posterior probability density function (pdf) is given by

$$P(\boldsymbol{\theta}, \boldsymbol{\beta}, \phi_{\mathbf{D}} | \tilde{\mathbf{D}}, \tilde{\mathbf{U}}, \phi_{\mathbf{U}}) \propto \mathcal{N}(\boldsymbol{\beta} | \mu_\beta, \sigma_\beta^2) P(\tilde{\mathbf{D}} | \boldsymbol{\theta}, \tilde{\mathbf{U}}, \boldsymbol{\beta}) P(\boldsymbol{\theta}) P(\phi_{\mathbf{D}}), \tag{.1}$$

where $\boldsymbol{\beta}$ is the vector of precipitation multipliers, $\tilde{\mathbf{D}}$ is a n-vector with streamflow observations, $\tilde{\mathbf{U}}$ is an input (forcing) data record ($n \times 2$ matrix with precipitation and potential evapotranspiration values), $\mathcal{N}(\cdot | \mu_\beta, \sigma_\beta^2)$ is the normal pdf with mean μ_β and variance, σ_β^2, and $\phi_{\mathbf{U}} = \{\mu_\beta, \sigma_\beta^2\}$ and $\phi_{\mathbf{D}}$ are latent variables of the uncertainty distributions of the input (rainfall) and output (streamflow) data, respectively.

If we now assume the streamflow data to have an additive Gaussian error with unknown variance, $\phi_{\mathbf{D}} = \sigma_{\mathbf{D}}^2$ then we yield the following formulation of the posterior pdf

$$P(\boldsymbol{\theta}, \boldsymbol{\beta}, \sigma_{\mathbf{D}}^2 | \tilde{\mathbf{D}}, \tilde{\mathbf{U}}, \phi_{\mathbf{U}}) \propto \mathcal{N}(\boldsymbol{\beta} | \phi_{\mathbf{U}}) \mathcal{N}\big(\tilde{\mathbf{D}} | \mathcal{F}(\boldsymbol{\theta}, \tilde{\mathbf{U}}, \tilde{\mathbf{x}}_0, \boldsymbol{\beta})\big) P(\boldsymbol{\theta}) P(\sigma_{\mathbf{D}}^2), \tag{.2}$$

where $\mathcal{F}(\cdot)$ signifies the forward model (HYMOD, SAC-SMA or TOPMO), and $\tilde{\mathbf{x}}_0$ denote the initial states - whose uncertainty is treated implicitly through the use of a spin-up period. Hence, explicit dependence of the posterior pdf on $\tilde{\mathbf{x}}_0$ is removed in the remainder of the derivation.

If we specify a Jeffrey's prior on the measurement error of the streamflow data, $P(\sigma^2_{\mathbf{D}}) \propto 1/\sigma^2_{\mathbf{D}}$ then we derive

$$P(\boldsymbol{\theta}, \boldsymbol{\beta} | \tilde{\mathbf{D}}, \tilde{\mathbf{U}}, \phi_{\mathbf{U}}) \propto \mathcal{N}(\boldsymbol{\beta}|\phi_{\mathbf{U}}) \mathrm{SS}_{\mathbf{D}}(\boldsymbol{\theta}, \tilde{\mathbf{D}}, \tilde{\mathbf{U}})^{-\frac{n}{2}}, \tag{.3}$$

where $\mathrm{SS}_{\mathbf{D}}$ is the sum of squared residuals between the observed and simulated discharge values

$$\mathrm{SS}_{\mathbf{D}}(\boldsymbol{\theta}, \tilde{\mathbf{D}}, \tilde{\mathbf{U}}) = \sum_{t=1}^{n} \left(\tilde{d}_t - \mathcal{F}(\boldsymbol{\theta}, \tilde{\mathbf{U}}, \tilde{\mathbf{x}}_0, \boldsymbol{\beta}) \right)^2 \tag{.4}$$

When little is known about the rainfall uncertainty, it is tempting to specify a noninformative prior on σ^2_β. If we assume the rainfall to be unbiased, on average, that is $\mu_\beta = 1$ and assume a Jeffrey's prior for σ^2_β, that is $P(\sigma^2_\beta) \propto 1/\sigma^2_\beta$, the following formulation of the posterior pdf is derived

$$P(\boldsymbol{\theta}, \boldsymbol{\beta} | \tilde{\mathbf{D}}, \tilde{\mathbf{U}}, \mu_\beta) \propto \mathrm{SS}_{\mathbf{U}}(\boldsymbol{\beta})^{-\frac{m}{2}} \mathcal{N}(\boldsymbol{\beta}|\phi_{\mathbf{U}}) \mathrm{SS}_{\mathbf{D}}(\boldsymbol{\theta}, \tilde{\mathbf{D}}, \tilde{\mathbf{U}})^{-\frac{n}{2}}, \tag{.5}$$

where $\mathrm{SS}_{\mathbf{U}}(\boldsymbol{\beta}) = \sum_{j=1}^{m} (\beta_j - \mu_\beta)^2$. Although this approach apparently incorporates a non-informative prior on the rainfall uncertainty, a careful attempt to explore Equation (.5) quickly runs into a fatal error: the posterior is unbounded whenever $\beta_j = \mu_\beta \, \forall \, j$, causing the inference to degenerate and become rather meaningless.

To stabilize (bound) the inference we have assume an informative prior for σ^2_β. For convenience, lets assume an inverse gamma prior on σ^2_β with shape parameter $\nu > 0$ and scale parameter $s_0 > 0$

$$P(\sigma_\beta^2|\nu, s_0) \propto \frac{1}{\sigma_\beta^{\nu+1}} \exp\left(-\frac{\nu s_0^2}{2\sigma_\beta^2}\right). \tag{.6}$$

If we combine this Equation with the likelihood of the input (rainfall) data we yield

$$P(\boldsymbol{\beta}, \sigma_\beta^2|\nu, s_0^2) \propto P(\sigma_\beta^2|\nu, s_0^2)P(\boldsymbol{\beta}|\sigma_\beta^2) \propto \frac{1}{\sigma_\beta^{\nu+1}} \exp\left(-\frac{\nu s_0^2}{2\sigma_\beta^2}\right) \frac{1}{\sigma_\beta^m} \exp\left(-\frac{\mathrm{SS}_{\mathbf{U}}(\boldsymbol{\beta})}{2\sigma_\beta^2}\right). \tag{.7}$$

Integrating this Equation over σ_β^2 and assuming a Gaussian distribution for the streamflow data error yields

$$P(\boldsymbol{\theta}, \boldsymbol{\beta}|\tilde{\mathbf{D}}, \tilde{\mathbf{U}}, \mu_\beta, \nu, s_0^2) \propto \left[\mathrm{SS}_{\mathbf{U}}(\boldsymbol{\beta}) + \nu s_0^2\right]^{-\frac{(m+\nu-1)}{2}} \mathrm{SS}_{\mathbf{D}}(\boldsymbol{\theta}, \tilde{\mathbf{D}}, \tilde{\mathbf{U}})^{-\frac{n}{2}}. \tag{.8}$$

This formulation is equivalent to the log-formulation in Equation 2.10 in the thesis. This concludes the derivation of the joint streamflow and precipitation data likelihood.