General Review of Rainfall-Runoff Modeling: Model Calibration, Data Assimilation, and Uncertainty Analysis

Hamid Moradkhani* **and Soroosh Sorooshian**

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1 Introduction

All Rainfall-Runoff (R-R) models and, in the broader sense, hydrologic models are simplified characterizations of the real world system. A wide range of R-R models are currently used by researchers and practitioners, however the applications of these models are highly dependent on the purposes for which the modeling is made. Many R-R models are used merely for research purposes in order to enhance the knowledge and understanding about the hydrological processes that govern a real world system. Other types of models are developed and employed as tools for simulation and prediction aiming ultimately to allow decision makers to take the most effective decision for planning and operation while considering the interactions of physical, ecological, economic, and social aspects of a real world system. Examples of some of the implications of latter type of R-R models are: real-time flood forecasting and warning, estimating flood frequencies, flood routing and inundation prediction, impact assessment of climate and land use change and integrated watershed management.

The development of R-R models could be recognized based on the importance of available data which provides the learning data set for calibrating the nonlinear behavior of these models. These data are used as a priori knowledge in the model with the logic that gives the flexibility to the model to extrapolate the R-R process for some future time. This line of thinking, known as batch model calibration (using batch of data for calibration), has been challenged by another philosophy that availability of observation continuously gives the opportunity to the model components (state variables and even parameters) to be updated (corrected) sequentially. This is thought to give more flexibility for taking advantage of the temporal organization

H. Moradkhani
Department of Civil and Environmental Engineering, Portland State University, Portland, OR, USA

* Work was completed while at the University of California, Irvine

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and structure of information content for better compliance of the model output with observed system response. The real time adjustment (fine-tuning) of R-R models for flood forecasting is categorized under the latter philosophy. In fact the need for on-line adjustments of R-R flood forecasting models was emphasized by WMO (1992).

2 Various Modeling Approaches: Lumped, Distributed and More

Owing to the complex nature of rainfall-runoff processes determined by a number of highly interconnected water, energy and vegetation processes at various spatial scales, hydrologists rely on their own understanding of the system gained through interaction with it, observation and experiments. This process is known as perceptual modeling (Beven, 2001). Perceptualization of a hydrologic system leads the modelers to a variety of ways to classify rainfall-runoff models from deterministic to stochastic models, from physically-based (white-box) to black-box or empirical and to conceptual models, and the most distinctive, from lumped models to distributed models (Clarke, 1973; Beven, 1985; Wheater et al., 1993; Refsgaard, 1996; Beven, 2001). In lumped models, the entire river basin is taken as one unit where spatial variability is disregarded. In such a modeling approach one tries to relate the forcing data, mainly precipitation inputs, to system outputs (streamflow) without considering the spatial processes, patterns and organization of the characteristics governing the processes. On the other hand, a distributed model is one which accounts for spatial variations of variables and parameters, thereby explicit characterization of the processes and patterns is made (Beven, 1985; Refsgaard, 1996; Smith et al., 2004). The history of lumped R-R models is traced back to the last century with the rational method which directly relates the precipitation input to the peak discharge through the runoff coefficient parameter. Due to some of the difficulties that this method causes (Beven, 2001), numerous complex lumped R-R models have been developed and documented (Fleming, 1975; Singh, 1995; Singh and Frevert, 2002a,b). The Crawford and Linsley's Stanford Watershed Model (1962) was one of the notably successful efforts in introducing a complex R-R model accounting for the dynamics of hydrologic processes governing in a watershed. The attempt by Crawford and Linsley (1962, 1966) was the first in benefiting from the digital computers for a quantitative description of the hydrologic processes. Other examples of conceptual R-R models are the Xinanjiang Model (Zhao et al., 1980), and the widely used operational model in the US National Weather Service (NWS) for flood forecasting, Sacramento Soil Moisture Accounting Model (SAC-SMA), developed by Burnash et al. (Burnash et al., 1973; Burnash, 1995).

The lumped hydrologic models impose many assumptions, especially in large watersheds, as variables and parameters are representative average values (lumped) for a river basin with semi-empirical equations describing the physics (Refsgaard, 1996). These models are generally designed to simulate the streamflow just at the watershed outlet. However, one may want to estimate the flow at some interior locations in a river basin for engineering design, for real time operational flood forecasting and also for studying the effects of land use or climate change. In general a rainfall-runoff model requires representing the interaction of surface and subsurface processes. Freeze and

Harlen (1969) were first to outline the underlying physics to describe such processes. The benefits of distributed models as outlined by Beven (1985) and summarized by Smith et al. (2004) are the possibility of considering spatially variable inputs and outputs, assessment of pollutants and sediment transport, and also analyzing the hydrological response at ungauged basins. The availability of high spatial resolution data such as DEM, precipitation, vegetation, soil and other atmospheric variables has led to a surge in developing many sophisticated distributed hydrologic models. As pointed out by Refsgaard (1996), in a distributed physically-based model the flows of water and energy fluxes are computed from the prevailing partial differential equations (e.g., Saint Venant equations for overland and channel flow, Richard's equation for unsaturated flow and Boussinesq's equation for groundwater flow). Several variants of distributed watershed models have been developed and implemented including SHE (Abbott et al., 1986a,b), TOPMODEL (Beven and Kirby, 1976, 1979), IHDM (Beven et al., 1987), THALES (Grayson et al., 1992), MIKE SHE (Refsgaard and Storm, 1995), KINEROS (Smith et al., 1995), HBV (Bergstrom, 1995); IHDM (Calver and Wood, 1995) to name a few.

The National Weather Service Hydrology Laboratory (NWS-HL) recently launched a Distributed Model Intercomparison Project (DMIP) to encourage collaborative research into appropriate levels of model complexity, value of spatially distributed data, and methods suitable for model development and calibration. This effort revealed the readiness of operational organizations to move towards distributed hydrologic modeling and the fact that they see the distributed modeling as a key pathway to infuse new science into their river and flash flood forecast operations and services (Smith et al., 2004; Koren et al., 2001). However, they are still facing the question that under what circumstances and for what type of forecasting, distributed modeling is profitable (Beven, 1985; Smith et al., 2004). Furthermore, if there is a justification to employ these complex models, which model is the best to improve the NWS forecasting capabilities?

The research community is facing some challenges in the application of the distributed models. There are still many outstanding questions regarding the parameterization, calibration, and error correction of these complex models. The estimation of the excessive parameters within distributed models is the main source of uncertainty in these models. Most of the studies on distributed modeling can be divided into two categories in regard to parameterization. Some studies propose certain assumptions to simplify the parameterization (e.g., Homogeneity or fixing some of the parameters, etc.) (Beven and Binley, 1992) and then to use calibration techniques to find optimal values for the rest of the parameters. The others take into account the heterogeneity that exists in the watershed and use soil and vegetation data to physically estimate the value of the parameters based on watershed characteristics within all the hydrologic units. In this case calibration is an intense, time consuming, and inefficient procedure due to the number of parameters involved.

These advantages motivated the National Oceanic and Atmospheric Administration's National Weather Service (NOAA/NWS) to initiate a distributed model intercomparison project (DMIP) to infuse new science and technology into its river forecasting capability Smith et al. (2004).

3 The Problem of Model Calibration (Parameter Estimation)

In general terms, hydrologic models are defined by state or prognostic variables which define the dynamics of a system, and also parameters as quantities characterizing the system. Parameters may be classified into physical and process parameters (Sorooshian and Gupta, 1995). Physical parameters are those which can be measured directly independent of the observable river basin responses, such as, watershed area, impervious area in a watershed, local permeability obtained using core samples, fraction of vegetated area, and areal percentage of water bodies. The process parameters, on the other hand, are those which can not be measured directly and needs to be inferred by indirect means (Gupta et al., 1998), such as, effective depth of soil moisture storage, effective lateral interflow, rate of drainage for hypothetical lumped storages, mean hydraulic conductivity, and surface runoff coefficient. Although these parameters cannot be expected to have physical interpretations, they are assumed to be related to inherent properties having physical relevance in hydrologic systems. In order for a model to closely and consistently simulate the observed response (dynamic behavior) of a river basin over some historical period for which forcing data (precipitation) and system output (e.g., streamflow) are available, the model parameters need to be tuned or calibrated. The linkage between data, model and parameters are shown schematically in Fig. 1. A variety of model calibration techniques have been developed and implemented to ensure conformity between the model simulations of system behavior and observations. A basic approach to obtain the parameter values is the trial and error procedure, the so called manual calibration. The model knowledge and large number of model performance measures defined by objective functions accompanied by visual inspection of the agreement and differences between model predictions and the observation, and above all, the human judgment are all taken to guide the adjustments to the best guess for model parameters (Boyle et al., 2000; Duan, 2003). There are 3 levels associated with

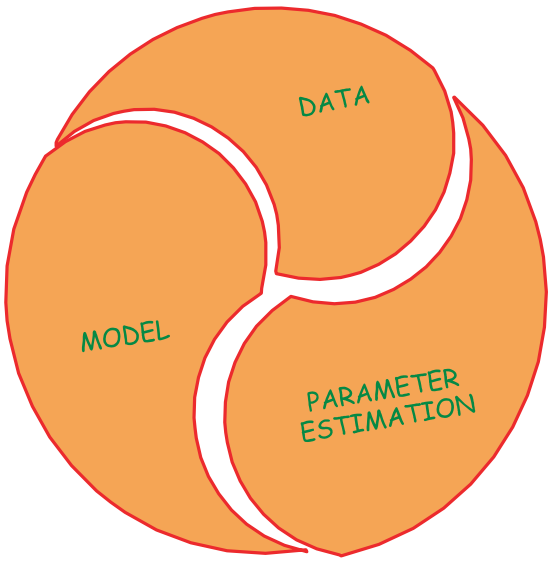

Fig. 1 Linkage of data, model and parameter estimation (calibration)

manual calibration (Boyle et al., 2000). In level zero, the watershed data are examined and a priori estimates of the likely values of parameter sets developed. This provides the initial uncertainty of the estimates by defining the feasible parameter ranges using the estimates from similar adjacent watersheds, look-up tables, etc. In level one, the analysis of some segments of streamflow hydrograph that are most relevant to specific parameter/s is made followed by the parameter adjustment. In this step, the parameter interaction is generally disregarded. Finally, in level two, the most difficult step, while examining the watershed hydrograph the parameter interaction is taken into account and adjustment of the parameters is made accordingly. The process of manual calibration is less affected by noises in calibration data; however, the multitude of nonlinearly interacting parameters in hydrologic models makes this procedure very labor-intensive requiring extensive training. This expertise is not only difficult to gain, but also hard to transfer from one hydrologist to another. These problems and difficulties justified the need for development of automatic calibration techniques (Sorooshian and Dracup, 1980; Sorooshian et al., 1993; Duan et al., 1992, 1993; Gupta et al., 1998; Hogue et al., 2000; Gupta et al., 2003a).

3.1 Mathematical Modeling of Hydrologic Systems

An R-R model can be cast in a mathematical framework irrespective of whether the model is physical, empirical and/or conceptual. In fact we are interested in mathematical models that simulate or predict outputs from inputs. We denote the R-R model by a nonlinear function $f(.)$ signifying the derivative of the state vector x with respect to time t. In addition, the system is characterized by k-member vector of parameters θ, and forcing field (input) variables u as follows:

$$\frac{dx_t}{dt} = f(x_t, \theta, u_t) + w_t \tag{1}$$

Where, $x_t \in \Re^{N_x}$ is an N_x-dimensional vector representing the system state (for example catchment soil moisture content) at time t. The nonlinear operator $f: \Re^{N_x} \rightarrow \Re^{N_x}$ expresses the system transition over a time instant in response to the model input vector (forcing data, u, e.g., mean areal precipitation). In regards with model parameters, it is further assumed that

$$\theta \in \Theta \subseteq \Re^k \tag{2}$$

Where, $\Re^k$ denotes the k-dimensional Euclidean space.

Due to error associated with the observed input to the system, the uncertainty in parameter estimation and/or parameter identification and also model structural error for accurate representation of physical data generating process, the aggregate uncertainty may be defined through an additive error term $w_t$which may consider to be white noise random sequence with mean zero and covariance Q_t.Considering that the hydrologic data are available at discrete time, the continuous differential

form in eq. (1) is written as following the discrete stochastic dynamic state-space form:

$$x_t = f(x_{t-1}, \theta, u_t) + w_t \tag{3}$$

Equation (3) is considered as an intermediate step to obtain the amount of internal storages and fluxes in a hydrologic system; however, the eventual goal in R-R modeling is to predict the output (runoff or streamflow) which are related to the model states through the following equation:

$$\hat{y}_t = h(x_t, \theta) \tag{4}$$

where, $\hat{y}_t \in \Re^{N_y}$ is an N_y-dimensional observation vector (observation simulation, e.g., streamflow) as a function of model parameters and forecasted state variables through the nonlinear operator $h : \Re^{N_x} \rightarrow \Re^{N_y}$.

Given the observed output values of y, the residual error term is written as:

$$v_t = y_t - \hat{y}_t \tag{5}$$

Combining eqs. (4) and (5) yields the standard formulation of observation equation:

$$y_t = h(x_t, \theta) + v_t \tag{6}$$

3.2 Inverse Methods

The mathematical formulation of the R-R system described in Section 3.1 is the typical Inverse Problem (IP) which could be explained as a problem where the input and output observations and sometimes state variables are known, but not the model parameters. Therefore, the problem of model calibration can be seen as the inverse problem. This is in contrast to a Forward Problem (FP) where the relevant properties of the model including initial and boundary conditions and also the parameters of the system are known. A model then predicts the states and outputs straightforwardly. Simply speaking, in FP, one wants to find effects (streamflow) from causes (parameters), while in IP, causes need to be found on the basis of effects. Unlike forward learning which is a many-to-one mapping problem, the inversion learning problem is one-to-many, therefore the mapping from output to input is generally non-unique. In other words, the same effects (streamflow) may be caused by different causes (parameters).

A problem is said to be well-posed if the three conditions for the solution are met according to the definition given by Hadamard (1990): existence, uniqueness and stability. According to this definition, the parameter estimation (model calibration) is an ill-posed problem due to non-uniqueness of the solution for model parameters (see Fig. 2). This is the typical case for inverse problems. The general formulation

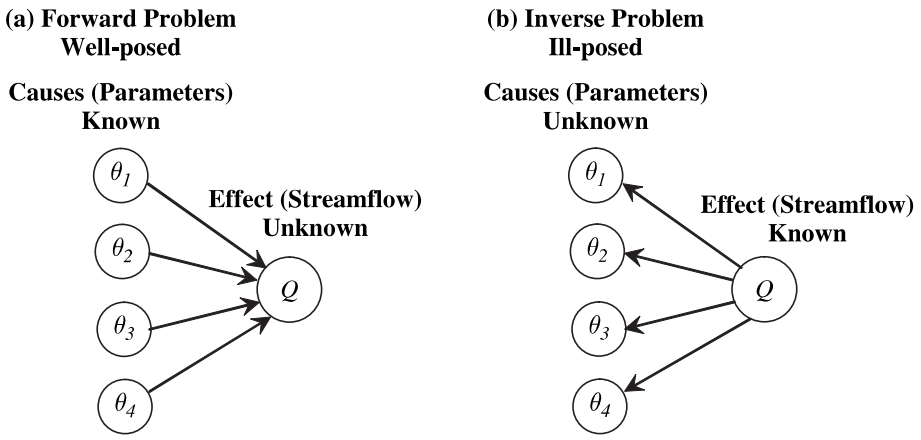

Fig. 2 Schematic of forward problem vs. Inverse problem

of the forward and inverse problems can also be shown as follows (Castelli and Entekhabi, 2002):

Consider a model $f(D, \theta) = [f_1(D, \theta), f_2(D, \theta), \ldots, f_L(D, \theta)]^T = 0$ Consisting of L elements which relates a data vector, $D = [d_1, d_2, \ldots d_N]^T$ and a parameter vector $\theta = [\theta_1, \theta_2, \ldots \theta_M]^T$. In R-R modeling the streamflow observation (Q) can be considered as data in such formulation. Therefore, FP is concerned with estimation (prediction) of the data D given the model f and the estimates of the model parameters θ. In IP, the concern is to estimate the model parameters θ given model f and observation of D.

In a statistical sense, IP can be considered as the parameter estimation problem. In such framework, the reliability and/or uncertainty of the estimation in addition to the parameter estimates can be derived.

3.3 Model Calibration as an Optimization Problem

The nonlinear relationship between the parameters and outputs of R-R models makes the linear regression solution methods impractical to use, thus reliance on iterative or sequential (recursive) procedures to attain an acceptable solution is required. Iterative schemes work by repeatedly computing the model accuracy based on the guessed model parameters and all available data. Iterative methods are necessarily restricted to off-line applications, where a batch of data has been previously collected for processing. In contrast, in sequential procedures, one uses each measurement (real system output) as soon as it becomes available to update the model parameters and model states which result in improved model outputs (Thiemann et al., 2001; Moradkhani et al., 2005a,b) This attribute makes such approaches practical in either on-line or off-line applications. In this section, we focus our attention to the batch automatic model calibration. Since the advent of digital computers, automatic model calibration through optimization methods has been used extensively to calibrate the conceptual R-R model parameters. In automatic calibration,

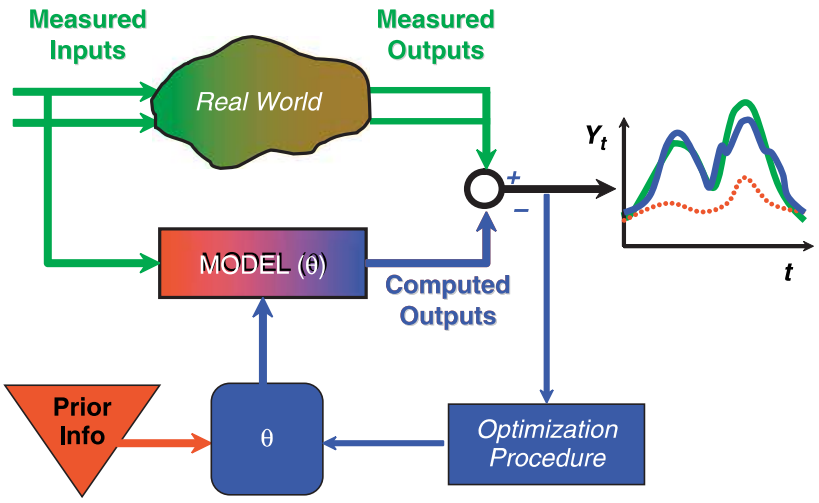

Fig. 3 The concept of model calibration as an optimization problem

the problem is formulated as an optimization problem through objective function or sometimes called loss or cost function (Fig. 3). This is a measure of the ability of the model to replicate the observed system response. The success of any model calibration depends on the observed data, model structure, calibration conditions and optimization procedure. Gupta et al. (2005) list the necessary conditions for a realistic hydrologic simulation by effectively estimating the model parameters called a well-calibrated model. These conditions are: (1) consistency of model structure and its behavior with current understanding of hydrologic processes, (2) consistency between input-state-output behavior of the model (as formulated in eqs. 1–6) and measurements of watershed behavior, (3) accuracy (unbiasedness) and precision (small uncertainty) of model predictions.

Early attempts for R-R model calibration have been made in 1960s and 1970s typically based on local search algorithms (Dawdy and O'Donnell 1965; Nash and Sutcliffe, 1970; Ibbitt, 1970). The local search methods are carried out by initialization of parameter sets and then iteratively minimizing the objective function to direct the parameter search towards local improvement. The local search methods are classified into direct methods (derivative-free) and gradient methods (derivative-based).

The rotating method of Rosenbrock (Rosenbrock, 1960), Pattern search (Hooke and Jeeves, 1961) and downhill simplex (Nelder and Mead, 1965) are examples of direct search methods. Gradient methods appear to be more powerful than direct methods as they use more information (including the first and second derivatives of objective function with respect to parameters) to obtain the optimum objective function (error response surface) value. The Newton and Quasi-Newton methods are examples of derivative-based local search methods. The local search methods for hydrologic model calibration have been reported by many others (Johnston and Pilgrim, 1976; Pickup, 1977; Gupta and Sorooshian, 1985; Hendrickson et al., 1988; among others) with the conclusion that local search methods cannot be used reliably to estimate the global optimal solution.

The philosophy behind any search algorithm in model calibration, random or nonrandom, for obtaining the best parameter set in the feasible range lies somewhere between exploration and exploitation. By exploration, one means to improve the objective function by randomly looking different regions of parameter space regardless of what has already been learned from previous sampling. An example of this type of parameter space search algorithm is uniform search. On the other hand, in exploitation the decision on how to sample the parameter space depends on the previous sampling. Examples of this type are the steepest descent and Newton-Raphson methods. The direct search Monte Carlo algorithms, such as importance sampling, falls somewhere between the exploration and exploitation methods. Better exploration and exploitation of response surface function to globally optimize the parameter sets was realized to be necessary owing to the existence of multiple local optima, discontinuous derivatives and multiple regions of attractions in the parameter space. Therefore, the attention geared towards global searching algorithms. This method should be able to not only cope with the aforementioned problems, they should be efficient and robust enough to overcome the problems that arise from the high dimensionality of parameter space in operational hydrologic models such as the SAC-SMA model and also the high degree of parameter interaction in such models. Examples of the global search methods are the Adaptive Random search (Masri et al., 1980; Brazil, 1988), Genetic algorithm (Holland, 1975; Goldberg, 1989; Franchini, 1996), Simulated Annealing (Kirkpatrick et al., 1983).

A novel global search approach called Shuffle Complex Evolution (SCE-UA) was introduced and implemented in a variety of hydrologic model calibration applications (Duan et al., 1992, 1993; Sorooshian et al., 1993). SCE-UA benefits from the strength of different procedures and combines their strategies including the Downhill Simplex, Controlled Random Search, and Competitive Evolution with the proposed idea of Complex Shuffling.

4 Ensemble Inference vs. Optimization

Despite the effectiveness, consistency and efficiency of some of the global optimization methods such as SCE-UA in reliably finding the global solution, numerous studies have shown that many combinations of parameter sets (while even widely distributed in parameter space) may result in similar objective function value, meaning that several optimum solutions may exist for a problem. This reveals the problem of nonuniqueness or nonidentifiability of parameters, the so-called equifinality (Beven, 1993) which is the cause of the existence of multiple feasible solutions for the same problem. This view suggests that there may exist many representations of a watershed (many possible parameter sets) that may be equally capable of simulating the observed system response and therefore rejects the concept of optimum parameter set despite the strong desire in environmental science in obtaining the single optimal representation of reality. Especially when the objective function in an optimization problem is highly irregular and nonlinear, multimodal

and nonsmooth with discontinuities, the global optimization procedures and matrix inversion may fail to converge to the optimum solution due to numerical instabilities caused by ill-conditioned matrices. To cope with these problems, Monte Carlo (MC) methods as ensemble inference may be employed. MC procedures work by direct sampling from the parameter space or associated probability distributions, they are not dependent on the objective function to be smooth nor do they suffer from numerical instabilities. MC methods based on the definition provided by Hammersley and Handscomb (1964) are considered as a branch of experimental mathematics that is concerned with experiments on random number. An up- to-date definition provided by Sambridge and Mosegaard (2002) states that MC methods are experiments making use of random numbers to solve either deterministic or probabilistic (stochastic) problems. Although MC methods originated as methods to solve the stochastic problems, later they were recognized as procedures to deterministic problems such as multidimensional integration (Arulampalam et al., 2002; Moradkhani 2004; Moradkhani et al., 2005b). The direct simulation of probability distributions can fundamentally be related to Monte Carlo methods. The use of MC methods in inverse problems as the information inference from measurement has garnered the attention of earth system scientists over the past decade. They may be used for inversion, parameter estimation, optimization, ensemble inference, and uncertainty assessment.

5 Hydrologic Uncertainties

Hydrologic prediction is highly influenced by the uncertainties in the forcing data (generally taken as deterministic), observed system response (due to errors in measuring the physical quantities), imperfection of the model structure and the parameter values resulting from the model calibration which is profoundly affected by uncertainty sources.

5.1 Uncertainty in Observation

The observation in R-R modeling is the measurement of the input and output fluxes of hydrologic system and even the storage in the system (states). The key to potential improvement of R-R modeling is associated with true characterization of precipitation uncertainty. Precipitation uncertainty is generally regarded as the most influential cause of uncertainty in flood forecasting. One of the early methods (*Bergestrom*, 1976) still used in an operational setting is to improve the model response by manually modifying the observed input and rerunning the model until there is a reasonable agreement between model output and observed runoff. Arguing about the validity of this approach is not the thrust of this chapter; however this shows that the main source of uncertainty in R-R modeling is the input (forcing data) uncertainty causing the significant effect on predictive uncertainty, not only due to the precision in

observation but due to the spatial and temporal averaging of these quantities. Therefore these fluxes need to be considered as stochastic quantities (Kavetski, 2003, 2006a,b; Clark and Slater, 2006; Hong et al., 2006; Moradkhani et al., 2006). As shown by Clark and Slater (2006), uncertainty in model simulation is strongly influenced by the reliability of the forcing variable and adequate characterization of their associated uncertainties. The role of input uncertainty becomes even more important for the ungauged regions or those regions where precipitation data are missing. In such cases, one may rely on remotely sensed precipitation products extracted from different satellite platforms. This will pose another challenge on how to estimate the error associated with the remotely-sensed product. Recently Hong et al. (2006) showed how the satellite precipitation error can be estimated through a power law function as follows:

$$\sigma_e = f(\frac{1}{L}, \frac{\Delta t}{T}, P) = a \cdot \left(\frac{1}{L}\right)^b \cdot \left(\frac{\Delta t}{T}\right)^b (P)^d \tag{7}$$

Where, σ_e is the error in precipitation (standard deviation between the satellite and radar data) which is a function of spatial coverage A (here substituted by L as spatial scale, the side length of A), temporal scale (T), satellite sampling frequency (Δt), and the space-time average of precipitation rate (P). $a, b, c,$ and d are the parameters of error model need to be calibrated. Also, Moradkhani et al. (2006) demonstrated how this error model can be used in conjunction with other uncertainty sources for the ensemble streamflow forecasting and how the interrelation of uncertainties through Particle Filtering (Moradkhani et al., 2005b) will result in combined streamflow uncertainty.

In addition to input data uncertainty, observed system response (streamflow) is subject to error reflected in the rating curve inaccuracies at very high and very low flows. This problem was addressed by Sorooshian and Dracup (1980), the problem known as heteroscedasticity (variance changing) of error with respect to the magnitude of flow as opposed to homoscedasticity (constant variance) of error.

5.2 Uncertainty in Parameter and State Estimation

As discussed earlier, significant consideration has been given to the development of automatic calibration methods aiming to successfully find a single best fitting parameter value; however less effort has gone into assessment of parameter uncertainty in hydrologic models. Therefore, despite the success of some of the global optimization methods such as SCE-UA, reliance on a "best" answer remains unrealistic due to the existence of many combinations of parameter sets in the feasible region. Poor identifiability of parameters may result in considerable uncertainty in model output. This problem may be resolved by means of ensemble inference through Monte Carlo procedures adopted by new generation of practitioners. Some of the available methods to estimate the parameter uncertainty using the ensemble inference are the Generalized Likelihood Uncertainty Estimation (GLUE) method

(Beven and Binley, 1992), the Bayesian Recursive Estimation (BaRE) algorithm developed by Thiemann et al., (2001); the Metropolis method reported by Kuczera and Parent (1998) and the Shuffled Complex Evolution Metropolis (SCEM-UA) algorithm of vrugt et al. (2003). The GLUE and SCEM-UA are implemented in a batch processing scheme where the collected period of data is used for calibration and uncertainty assessment; however as Gupta et al. (2005) reported, the GLUE can be applied recursively by choosing an appropriate likelihood function. The GLUE method works based on different realization of parameter sets in order to estimate the sensitivity of model prediction to various parameter sets. By doing so, the parameter sets are categorized into behavioral and non-behavioral via a likelihood measure. Those that are considered as non-behavioral are discarded for prediction. The recent study by Mantovan and Todini (2006), however, reported the reduced capacity of this method owing to its inconsistency with the Bayesian inference process leading to large overestimation on uncertainty, both for the parameter estimation and hydrologic forecasting uncertainty assessment. The BaRE algorithm employs a sequential approach to derive the probabilities associated with parameter sets in an on-line fashion. The parameter probabilities result in probabilistic output (streamflow) prediction. The problem with the original BaRE algorithm (Beven and Young, 2003; Gupta et al., 2003b) was its tendency to collapse onto a single point, a drawback modified by Misirli et al. (2003) through a resampling procedure. The Metropolis method of Kuczera and Parent (1998) for the parameter uncertainty estimation uses a random walk in the parameter space that adapts to the true probability distribution of parameters. The underlying idea in the MH method as a MCMC algorithm is generating samples of a probability distribution over a high dimensional space where no explicit mathematical expression exists for the probability distribution. The SCEM-UA is the extension of the SCE-UA algorithm (Duan et al., 1992) with the difference that the Downhill Simplex method which was used for population evolution in SCE-UA was replaced by the Metropolis Hastings (MH) algorithm in SCEM-UA. The usage of MH keeps the SCE-UA solution from collapsing into a single point (global optimum) in parameter space; this is due to the stochastic nature of MH as a Markov Chain Monte Carlo (MCMC) procedure.

Another procedure to modify parameters and estimate the uncertainty associated with them is real time calibration via filtering techniques. Recursive estimation based upon Kalman filter-type algorithms are generally used for estimating the dynamic state of the system. However, as several authors have reported, the real time updating of state variables and parameter values is essential allowing the model to more closely reproduce the observed system response due to the updating criteria carried out in each observation time. (Todini, 1976, 1978; Kitanidis and Bras, 1980a,b; Georgakakos, 1986a,b; Rajaram and Georgakakos, 1989; Georgakakos and Smith, 1990; Kivman, 2003; Moradkhani et al., 2005a,b). The real-time calibration using the Extended Kalman Filter (EKF) for the operational SACramento Soil Moisture Accounting Model (SAC-SMA) proposed by Georgakakos (1986a,b) was investigated by WMO (1992) and concluded that the approach should not be recommended because of its instability of parameter estimates (as a result of linearization of the

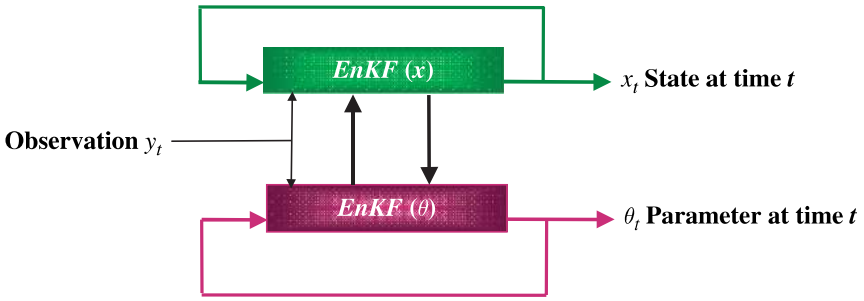

Fig. 4 Dual State-parameter estimation using Ensemble Kalman Filter (EnKF)

system) and also computational requirements of implementing of such system. The recent development by Moradkhani et al. (2005a) on dual state-parameter estimation (see the schematic in Fig. 4) showed how the drawback of previous approaches could be overcome while using the Ensemble Kalman Filter (EnKF). In such an approach, multiple possible model realization including parameters and state variables, while incorporating the input uncertainty for generating the model replicates, are used and the states and parameters are updated by the availability of observation.

6 Bayesian Inference and Sequential Data Assimilation

In the optimization methods, estimates of error are not readily available while Bayesian inference provides a mechanism to combine the quantitative (hydrologic data) and qualitative (prior information obtained by the experience of experts in the field) data to yield the posteriori as more informative probability distribution of variable of interest.

Bayesian formulation allows hydrologists to estimate the uncertainty about prediction in a meaningful way and can be accomplished without resort to calibration which is sometimes problematic in certain applications. However, as shown by Thiemann et al. (2001), vrugt et al. (2003) and Moradkhani et al. (2005a,b), calibration as a paramount element in hydrologic prediction can be made within the Bayesian paradigm.

In fact, in a Bayesian formulation, the solution to an inverse problem is given by posterior probability distribution $P(M|D)$ over the model space. $P(M|D)$ encompasses all the available information on model which are taken from both data (D) through the likelihood function $P(D|M)$, and also data-independent prior information expressed by prior probability $P(M)$density. The mathematical description of Bayes law is given in below:

$$P(M|D) = \frac{P(D|M)P(M)}{P(D)} \tag{8}$$

Where the denominator, $p(D)$ is the normalization factor, i.e., it ensures that the integration of $p(M|D)$ results to 1. The likelihood function $p(D|M)$ which measures

the likelihood of a given model Mthrough its misfit $e(.)$,the error between observation and model simulation, is given in general form as follows:

$$p(D|M) \propto exp(-e(.)) \tag{9}$$

With the assumption that the model residuals are mutually independent, normally distributed, with constant variance (i.i.d.), the likelihood function can be computed using (Box and Tiao, 1973):

$$p(D|M) \propto \exp\left[-\frac{1}{2}\sum\left(\frac{e(.)}{\sigma}\right)^2\right] \tag{10}$$

In the absence of an explicit mathematical expression for $P(D|M)$ and$P(M)$, which is common in high dimensional problems, Monte Carlo sampling is used to explore posterior $P(M|D)$. The importance sampling, Metropolis-Hastings algorithm and Gibbs Sampler are the most commonly used sampling techniques in practice.It should be noted that the sampling should not be biased toward any particular region of parameter space and thereby no possibility of entrapment in local minima.

The original Bayes law explained above eq. (8) is in the batch form where the available historical data is taken for the uncertainty estimation through that conditional probability. However, this form makes no attempt to include information from new observations when becoming available. The flexibility required to use the new information is provided by a sequential Bayesian scheme. Moradkhani et al. (2005a,b) showed that the methods based on sequential Bayesian estimation seem better able to benefit from the temporal organization and structure of information achieving better conformity of the model output with observations.

If we consider the state variable x_t as the variable of interest to be estimated within the Bayesian framework, because of its stochastic nature, the pertinent information about it at time t can be extracted from the observation $Y_t = [y_1, y_2, \ldots y_t]$ through the recursive Bayes law:

$$p(x_t|Y_t) = p(x_t|y_t, Y_{t-1}) = \frac{p(y_t|x_t)p(x_t|Y_{t-1})}{p(y_t|y_{1:t-1})} = \frac{p(y_t|x_t)p(x_t|Y_{t-1})}{\int p(y_t|x_t)p(x_t|Y_{t-1})dx_t} \tag{11}$$

As seen in the schematic of recursive Bayes law (Fig. 5), the forecast density of $p(x_t|y_{1:t-1})$ can be estimated via Chapman-Kolmogorov equation (Jazwinski, 1970) considering the Markovian property of order one holds in eq. (3), therefore:

$$p(x_t|Y_{t-1}) = \int p(x_t|x_{t-1})p(x_{t-1}|Y_{t-1})dx_{t-1} \tag{12}$$

The main complication in using the recursive Bayes law is that the multidimensional integration of forecast density as shown in eq. (12) makes the closed form solution of eq. (11) intractable. Therefore, reliance on ensemble methods through the Monte Carlo sampling is required, which makes such problems solvable in practice. In the

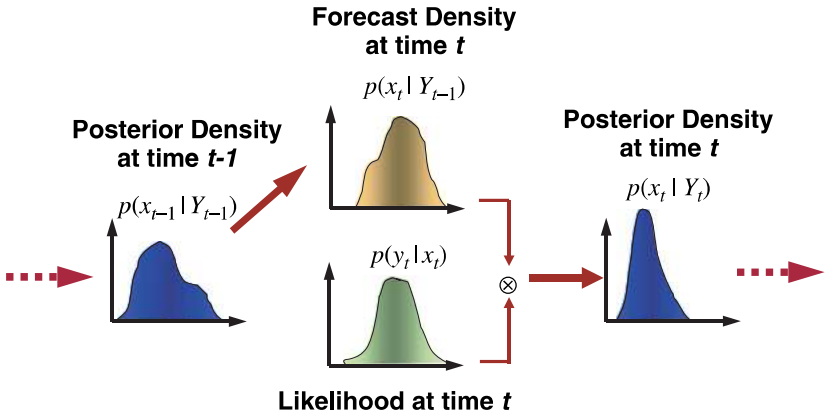

Fig. 5 Sequential Bayesian scheme for evolution of the conditional probability density of the state variables by assimilating observations from time t–1 to time t

next section we will explain how the conditional distribution of variable of interest can be estimated using the sequential ensemble filtering.

6.1 Ensemble Filtering

The aim of filtering is to use the observations Y_t over the time interval [0,t] to improve the current state x_t of a system. Two sequential estimation operations are discerned in filtering applications: (1) the forecasting step which is the transition of state variables from one observation time to the next as shown in eqs. (1) and (3) and probabilistically represented through transition probability $p(x_t|x_{t-1})$ in eq. (12), (2) the analysis (updating) step which involves updating of the forecasted (propagated) states with the new observation. Ensemble procedures present a practical alternative to an exact Bayesian solution by relying on discrete estimation of forecast (priori) and analysis (posteriori) densities through a set of random variables and corresponding weights:

$$p(x_t|Y_{t-1}) \approx \sum_{i=1}^{N} w_t^{i-} \delta(x_t - x_t^{i-}) \tag{13}$$

$$p(x_t|Y_t) \approx \sum_{i=1}^{N} w_t^{i+} \delta(x_t - x_t^{i+}) \tag{14}$$

These are the empirical approximation of forecast and analysis densities by summation of N Dirac delta functions where x^i and w^i denote the *ith* sample and its weight before and after updating shown by minus and plus signs respectively. The random replicates and associated weights are generated through a variety of methods, two of which are the ensemble Kalman filter (EnKF) and the Particle filter (PF). The

forecasting step in both EnKF and PF is the same where the evolution of the model for each ensemble member is equally weighted.

$$x_t^{i-} = f(x_{t-1}^i, \theta, u_t^i) \tag{15}$$

$$w_t^{i-} = \frac{1}{N} \tag{16}$$

Thereby, the forecast density will be as follows:

$$p(x_t|Y_{t-1}) \approx \frac{1}{N} \sum_{i=1}^{N} \delta(x_t - x_t^{i-}) \tag{17}$$

It is noted that in this process, the random input replicates of u_t^i are required to generate the state trajectories in eq. (15). One way to generate the input replicates is to consider the standard error obtained from eq. (7) and generate the random variable using the Gaussian distribution as illustrated in Moradkhani et al. (2006).

If the dynamical system, including states and measurement equations, are linear and all sources of uncertainty are normally distributed, the celebrated Kalman filter (Kalman, 1960) provides the optimal recursive solution to the state updating problem. If the system is nonlinear, as is the case for most of the hydrologic systems, the linearization of the system might be considered. Developed from the early work using state-space filtering, Georgakakos and Sperflage (1995) implemented an automatic procedure into the NWSRFS using the EKF. Certain shortcomings of the procedure have been discovered including: reformulation of the original SAC-SMA model to a state-space form; using first order approximation of Taylor series which leads to unstable results when the nonlinearity in the model is strong; and heavy computational demands owing to error covariance propagation. To overcome the limitation of the EKF, the EnKF was introduced by Evensen (1994) which was used for assimilating data in large nonlinear ocean and atmospheric model. The EnKF is also based upon Monte Carlo or ensemble generations where the approximation of the forecast state error covariance matrix is made by propagating an ensemble of model states using the updated states from the previous time step. The key point in the performance of the EnKF is to generate the ensemble of observations at each update time by introducing noise drawn from a distribution with zero mean and covariance equal to the observational error covariance matrix; otherwise the updated ensemble will possess a very low covariance (Moradkhani et al., 2005a).

$$x_t^{i+} = x_t^{i-} + K_t(y_t^i - \hat{y}_t^i) \tag{18}$$

$$K_t = \sum\nolimits_t^{xy-} \left[\sum\nolimits_t^{yy} + \sum\nolimits_t^{vv} \right]^{-1} \tag{19}$$

where $\sum_t^{yy}$ is the forecast error covariance matrix of the prediction $\hat{y}_t^i = h^i(.)$, $\sum_t^{xy-}$ is the forecast cross covariance of the state variables x_t^{i-} and prediction $\hat{y}_t^i$ and $\sum_t^{vv}$ is the observation error covariance of v in eq. (6).

If it is assumed that the forecast and measurement are jointly normal, their densities are sufficiently characterized by their mean and covariances, meaning that the higher order moments can be ignored in the update step.

As pointed out and implemented by Pham (2001), Arulampalam et al. (2002) and Moradkhani et al., (2005b), to improve the estimation accuracy and stability, one may want to track the time evolution of the model by means of all moment characteristics through a full probability density function. This is facilitated by using particle filters. If we use the particle filtering for the updating step, the updated ensemble members (particles) are kept the same as the forecast values and only the weights are updated. Therefore,

$$x_t^{i+} = x_t^{i-} \tag{20}$$

and from eq. (11), the filtering posterior, w_t^{i+} is calculated as follows:

$$w_t^{i+} = M.p(y_t|x_t^{i-})w_t^{i-} = \frac{M}{N}p(y_t|x_t^{i-}) \tag{21}$$

where, M is the normalizing constant in eq. (21). The important issue in using the particle filters is the sampling concept through different methods such as the Sequential Importance sampling (SIS), Sequential Importance Resampling or Sampling Importance Resampling (SIR) as the most commonly used sampling procedures. Using the proper sampling technique keeps the particles from dispersion due to stochastic behavior of the system or degeneracy which is the collapsing of all particles to a single point. For detailed information on particle filter and the sampling techniques, see Moradkhani et al., (2005b).

In general filtering is used to recursively estimate the posterior distribution of the model state; however, the successful use of sequential data assimilation relies on unbiased model state prediction, which is largely dependent on accurate parameter estimation (Moradkhani et al., 2005a,b). Moradkhani et al., (2005b) extended the application of the Bayesian recursive technique within the Monte Carlo framework for adaptive inference of the joint posterior distribution of the parameters and state variables within the sequential ensemble filtering. The use of this methodology relaxes the need for restrictive assumptions regarding the variables' probability density function; i.e., it can handle the propagation of non-Gaussian distribution through a nonlinear model properly. It provides a platform for improved estimation of hydrologic model components and uncertainty assessment by complete representation of forecast and analysis probability distributions. In Fig. 6 the schematic of joint Bayesian recursive estimation as the extension of Bayesian state estimation approach is displayed.

Figure 7 shows an example of how such a system can produce a probabilistic state-parameter estimate for ensemble streamflow forecasting. In Fig. 5, the

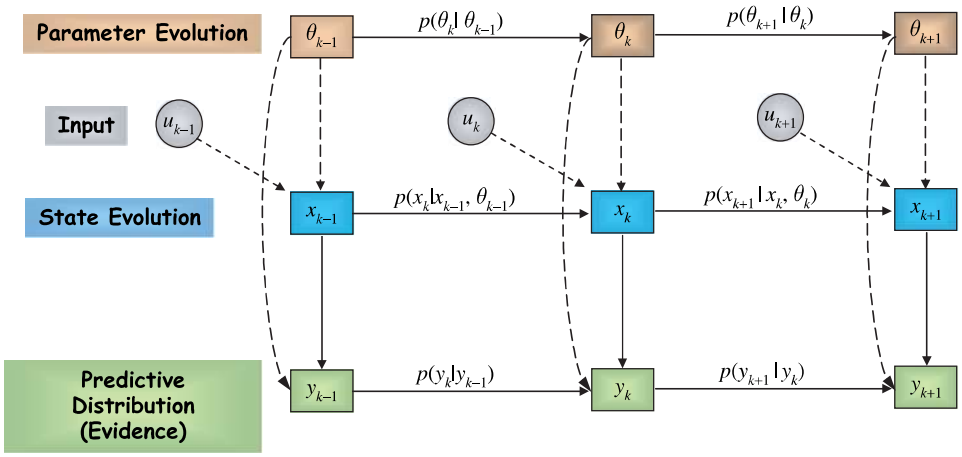

Fig. 6 Schematic of combined Bayesian filtering for state-parameter estimation

evolutions of the uncertainties associated with one model parameter, one state variable, and the streamflow output are displayed. Shaded areas in subplot (a) correspond to 95, 90, 68 and 10 percentile confidence intervals. Also gray areas in subplots (b) and (c) are associated with 95 percentile confidence interval with the mean of ensembles shown by solid line, while the cross marks in (c) represent the actual observation.

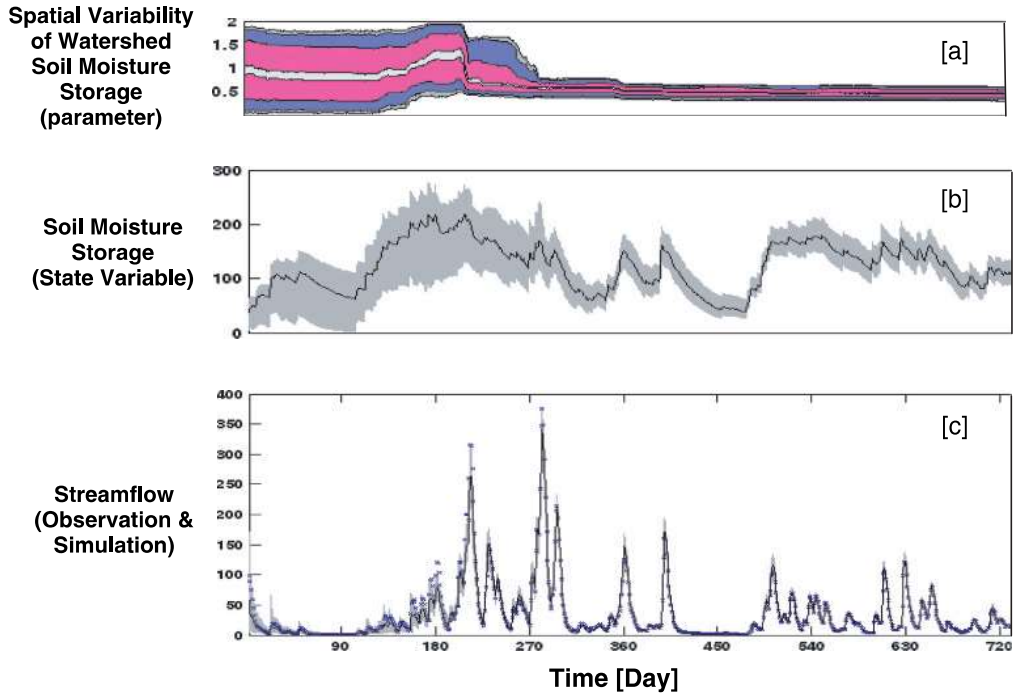

Fig. 7 Uncertainty bound evolution of hydrologic model components resulting in the ensemble (probabilistic) streamflow prediction

7 Summary

In this chapter, the brief description of rainfall-runoff models was placed into perspective with some history and background on various modeling approaches with the premise that the rainfall-runoff models are lumped or distributed conceptualization of the real-world system. The main elements of conceptual models were discussed and the mathematical configuration of a hydrologic system was illustrated followed by the simple input-state-output characterization of a system. This structure was put into a mathematical context. The concept of model calibration (parameter estimation) as an inverse problem was reviewed and the historical enhancement of calibration procedures were elaborated. While discussing the values of optimization techniques as objective approaches to do the automatic calibration, the concept of ensemble inference as an alternative to optimization of model performance was illustrated. Especially when the objective function in an optimization problem is highly irregular and nonlinear, multimodal and nonsmooth with discontinuities, the global optimization procedures and matrix inversion may fail to converge to the optimum solution due to numerical instabilities caused by ill-conditioned matrices. To cope with these problems, Monte Carlo (MC) methods as ensemble inference may be employed. The sources of uncertainties in hydrologic prediction were briefly discussed and it was shown how the Bayesian inference and the sequential data assimilation can be used for simultaneous calibration and uncertainty estimation. The ensemble filtering, mainly ensemble Kalman filter and particle filter, within the Bayesian paradigm were explained and a simple application was demonstrated.

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