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# Effect of heteroscedasticity treatment in residual error models on model calibration and prediction uncertainty estimation

Ruochen Sun [a], Huiling Yuan [a,b,*], Xiaoli Liu [c]

[a] School of Atmospheric Sciences and Key Laboratory of Mesoscale Severe Weather/Ministry of Education, Nanjing University, Nanjing, China
[b] Joint Center for Atmospheric Radar Research of CMA/NJU, China
[c] School of Engineering, Anhui Agricultural University, Hefei, China

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ABSTRACT

The heteroscedasticity treatment in residual error models directly impacts the model calibration and prediction uncertainty estimation. This study compares three methods to deal with the heteroscedasticity, including the explicit linear modeling (LM) method and nonlinear modeling (NL) method using hyperbolic tangent function, as well as the implicit Box-Cox transformation (BC). Then a combined approach (CA) combining the advantages of both LM and BC methods has been proposed. In conjunction with the first order autoregressive model and the skew exponential power (SEP) distribution, four residual error models are generated, namely LM-SEP, NL-SEP, BC-SEP and CA-SEP, and their corresponding likelihood functions are applied to the Variable Infiltration Capacity (VIC) hydrologic model over the Huaihe River basin, China. Results show that the LM-SEP yields the poorest streamflow predictions with the widest uncertainty band and unrealistic negative flows. The NL and BC methods can better deal with the heteroscedasticity and hence their corresponding predictive performances are improved, yet the negative flows cannot be avoided. The CA-SEP produces the most accurate predictions with the highest reliability and effectively avoids the negative flows, because the CA approach is capable of addressing the complicated heteroscedasticity over the study basin.



## 1. Introduction

Advances in hydrologic models in recent years have led to an increasing need to improve calibration and generate realistic prediction intervals (Stedinger et al., 2008), for the applications of short-term flood warning and long-term water resource management. Probabilistic uncertainty quantification has now become essential practice (Evin et al., 2014; Stedinger et al., 2008) for both research and operational modeling, e.g., during forecasting and parameter regionalization (Zhang et al., 2008).

Research on probabilistic uncertainty analysis has mainly two general approaches, including: (1) using residual error models to treat total uncertainty in a lumped manner (e.g., Bates and Campbell, 2001; Evin et al., 2013, 2014; Schoups and Vrugt, 2010; Sorooshian and Dracup, 1980); (2) separating predictive uncertainty into its contributing sources (e.g., Giudice et al., 2013; Gotzinger and Bardossy, 2008; Reichert and Mieleitner, 2009; Renard et al., 2010). Errors in input, model structural, output, and parameters are typically lumped into the residual errors for the former approaches, which are conceptually simpler for operational applications (e.g., Tuteja et al., 2011) and less data intensive than the latter approaches (Evin et al., 2014). This study focuses on the residual error model approaches, in which model parameter estimates are based on a likelihood function quantifying the probability that the measured data are reproduced by a particular parameter set (Box and Tiao, 1992). Therefore, adequately characterizing the form of residual errors is of great importance to obtain reliable and precise parameter distributions and hydrologic predictions.

However, due to the complexity of physical processes and the deficiencies in the hydrologic models, residual errors often show characteristics of autocorrelation, nonnormality and heteroscedasticity (Sorooshian and Dracup, 1980). Consequently, assumptions about the residual errors are most likely violated in many hydrological applications (Cheng et al., 2014; Leta et al., 2015; Nourali et al., 2016; Schoups and Vrugt, 2010). The autocorrelation can be represented using the autoregressive (AR) models (Bates and Campbell, 2001; Li et al., 2015, 2016; Schaefli et al., 2007; Sorooshian and Dracup, 1980) or the more general autoregressive

* Corresponding author at: School of Atmospheric Sciences and Key Laboratory of Mesoscale Severe Weather/Ministry of Education, Nanjing University, Nanjing 210023, China.
*E-mail address:* yuanhl@nju.edu.cn (H. Yuan).

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moving average (ARMA) model (Kuczera, 1983). The nonnormality of residual errors is often addressed by using data transformation methods (Box and Cox, 1964; Krzysztofowicz, 1997; Romanowicz et al., 1994; Wang et al., 2012) or can be explicitly represented by different probability distributions (Marshall et al., 2006; Schaefli et al., 2007; Schoups and Vrugt, 2010).

As for heteroscedasticity, implicit transformational methods can also be used to stabilize variance. For example, Box-Cox transformations have been widely used to transform streamflow and hold great potential to deal with the strong heteroscedasticity (Engeland et al., 2010; Laloy et al., 2010; Li et al., 2011; Smith et al., 2015). However, their primary goal is to transform non-Gaussian distributions to near-Gaussian shape. Besides, Box-Cox transformations fail to characterize heavy-tailed residuals, as shown in the studies of Bates and Campbell (2001) and Yang et al. (2007a). Compared to the implicit transformation methods, heteroscedasticity can be represented explicitly by conditioning the standard deviation of residual errors on explanatory variables such as streamflow. The most common method is to describe the standard deviation of residuals as a linear function of streamflow (Evin et al., 2013; Thyer et al., 2009; Schoups and Vrugt, 2010; Yang et al., 2007b). Evin et al. (2013) further pointed out that applying a linear model to standardize raw residuals, followed by the application of a first order AR (AR(1)) model to the standardized residuals, will lead to more reliable probabilistic prediction. In addition to the linear heteroscedastic model, Wang et al. (2012) derived the log-sinh transformation by assuming a nonlinear model between standard deviation of residual errors and streamflow.

In this study, autocorrelation, nonnormality and heteroscedasticity of residual errors were all considered in the model calibration and uncertainty estimation process. The autocorrelation was accounted for by applying an AR(1) model to the standardized residuals, based on Evin et al. (2013). For processing the nonnormality of residual errors, the skew exponential power (SEP) distribution (Schoups and Vrugt, 2010) which has flexible form and is easily adapted for normal distribution, was applied. Few studies have focused on the advantages and disadvantages of implicit transformational methods and explicit methods for dealing with heteroscedasticity. To compare the effect of the heteroscedasticity treatment in residual error models, three traditional methods of treating the heteroscedasticity were applied in this study, including two explicit methods: linear modeling (LM) and nonlinear modeling (NL) using hyperbolic tangent function, as well as one implicit method: Box-Cox transformation (BC).

The heteroscedasticity becomes stronger and more complicated for large heterogeneous river basins with complex climate conditions and strong seasonality, which poses great challenges for the application of traditional methods to deal with heteroscedasticity. Evin et al. (2014) pointed out that the error heteroscedasticity was poorly represented by a linear model in ephemeral catchments. McInerney et al. (2017) compared different approaches for representing error heteroscedasticity in different basins and found that predictive performance in ephemeral catchments was typically worse than other catchments. Therefore, the aim of this study is to assess different heteroscedasticity treatment methods of residual errors in a large basin with complex climate conditions and strong seasonality. A case study was conducted using the Variable Infiltration Capacity (VIC, Liang et al., 1994, 1996) hydrologic model over the Huaihe River basin of China, where sharp shift of flood and drought often occurs (Sun et al., 2016) and the error characteristics are similar to ephemeral catchments.

Based on the results of three residual models of treating heteroscedasticity applied in the VIC model, the streamflow predictions were not satisfying enough over the Huaihe River basin. Therefore, we proposed a combined approach (CA) combining BC with LM trying to deal with the strong and complex heteroscedasticity. In conjunction with the SEP distribution and the AR(1) model, four residual models (LM-SEP, NL-SEP, BC-SEP, and CA-SEP) were generated and their corresponding likelihood functions were adapted from the generalized likelihood (GL) function in Schoups and Vrugt (2010). The ultimate objectives are to identify the impacts of these residual error models on capturing the skewness and kurtosis of residual errors, avoiding negative flows, and producing reliable probabilistic predictions.

The rest part of the paper is organized as follows. Section 2 introduces the four residual error models employed in the study. Section 3 describes the study area and various data, as well as detailed methodology including hydrologic model calibration method and verification methods. Results are provided in Section 4, followed by discussions and conclusions in Section 5.

## 2. Residual error models

### 2.1. Bayesian inference

A residual error model is used to describe the residual errors $e_t$, defined as

$$e_t = \tilde{Q}_t - Q_t(\theta_H) \tag{1}$$

where $\tilde{Q}_t$ is the observed streamflow at time step t and $Q_t\ (\theta_H)$ is the simulated streamflow with hydrologic parameters $\theta_H$ at time step t.

According to Bayes theorem, the posterior distribution of parameters is

$$p(\theta_H, \theta_e | \tilde{Q}) \propto p(\tilde{Q}\,|\theta_H, \theta_e) p(\theta_H, \theta_e) \tag{2}$$

where $\theta_e$ denotes the residual error model parameters, $p(\tilde{Q}\,|\theta_H, \theta_e)$ is the likelihood function and $p(\theta_H, \theta_e)$ is the prior distribution of hydrologic and residual error model parameters. The likelihood function can be represented in the form of the joint probability density function (PDF) of the residuals

$$p(\tilde{Q}\,|\theta_H, \theta_e) = p(e[\theta_H]|\theta_e) \tag{3}$$

where $e[\theta_H]$ is the vector of residual errors obtained over the calibration period.

### 2.2. Formulations

In this study, we have examined four residual error models for model calibration and streamflow prediction. All residual models apply the AR(1) model to the normalized residual errors, which can lead to more reliable predictive performances as shown by Evin et al. (2013). In addition, the innovations follow the assumption of Evin et al. (2014) to have a unit variance, which will facilitate parameter estimation.

The differences among the four models mainly lie in the approaches to deal with heteroscedasticity, as shown in Table 1. Both the explicit method and the implicit method are tested. In addition, a new approach which combines LM with BC, is introduced.

1. LM-SEP. This residual error model is similar to the GL error model except that the AR(1) is applied to the standardized residuals based on Evin et al. (2013), which is defined by

$$\eta_t = \frac{e_t}{\sigma_t};\ \eta_t = \varphi_1 \eta_{t-1} + a_t \text{ with } a_t \sim SEP(0, 1, \xi, \beta);\ \sigma_t = \sigma_0 + \sigma_1 Q_t \tag{4}$$

where $\sigma_t$ is a normalization term, $\varphi_1$ is the first-order autoregressive coefficient and $a_t$ is the innovation described by the SEP