

# Bayesian total error analysis for hydrologic models: Sensitivity to error models

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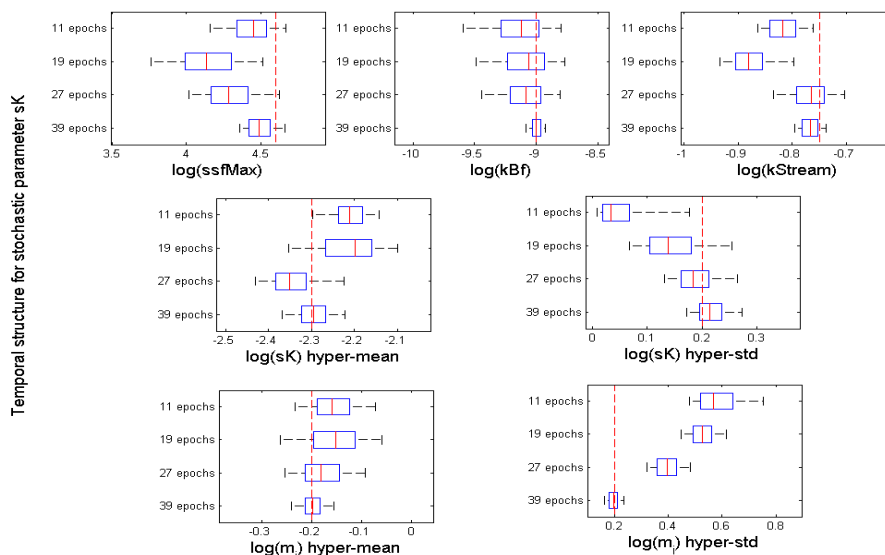
## EXTENDED ABSTRACT

The Bayesian Total Error Analysis methodology (BATEA) offers a robust approach to deal with the structural error of the model conceptualisation and measurement uncertainty in forcing/response data in conceptual rainfall-runoff (CRR) models. The core idea is to pose the model calibration as a Bayesian hierarchical model with latent variables describing errors in the data and the CRR model. The results from this calibration approach produced a dramatic shift in the parameter values compared to classical least squares calibration. This has considerable potential to enhance the regionalisation of hydrological model parameters. However for regionalisation to occur, a key issue is the selection of suitable probability models for latent variables, including the choice of the hyperdistribution and the choice of the time scale used to define latent variables.

This paper explores this issue using synthetic case studies. Synthetic data corrupted by various input

and structural errors are generated from the LogSPM CRR model. These data are then used to calibrate parameters using BATEA models derived with various hypotheses regarding the probabilistic properties of latent variables. Comparison of the parameter values between different approaches illustrate how sensitive the parameters are to different probability models.

Several conclusions can be drawn from this study. First, parameter estimates are more sensitive to the temporal structure used to model input errors than to the chosen hyperdistribution. Second, using latent variables of rainfall errors defined on a daily basis leads to more robust estimates than a storm epoch-based definition. Lastly, parameter estimates were found to be robust in the presence of structural error misspecification. This robustness is achieved through an artificial increase of input error variance, which compensates for unaccounted structural errors (Figure 1).



**Figure 1.** Marginal posterior distributions of three deterministic CRR parameters, and hyperparameters of stochastic parameter  $sK$  and rainfall errors, as a function of the temporal structure used to define latent variables of  $sK$ .

## 1. INTRODUCTION

Rigorous quantification of the uncertainties arising during the calibration of conceptual rainfall-runoff (CRR) models remains a challenging task in hydrological modelling. Several promising approaches have recently emerged in order to account for various sources of errors (Vrugt *et al.*, 2005, Ajami *et al.*, 2006, Vrugt and Robinson, 2007). The Bayesian total error analysis (BATEA) methodology has been proposed as a general framework to deal with the structural error of the model conceptualisation and measurement uncertainty in forcing/response data (Kavetski *et al.*, 2006a, b). The core idea is to pose the model calibration as a Bayesian hierarchical model with latent variables describing errors in the data and the CRR model. However, a key issue is the selection of suitable probability models for these latent variables.

This paper explores the sensitivity of BATEA estimates to the choice of latent variable probability models. It is organized as follows: first the general formulation of BATEA is reviewed. Then a range of latent variable probability models are described for assessment in the BATEA framework. The sensitivity of BATEA inference to misspecification of the probability models is then evaluated. These results are used to provide guidelines about the derivation of robust error models.

## 2. BATEA INFERENCE

### 2.1. Notation and hypotheses

The following notation will be used throughout this paper to denote data and variables involved in CRR model calibration.  $\mathbf{Q} = (q_t)_{t=1, \dots, T}$  denotes the true outputs of the model (e.g. runoff). For simplicity, we will only consider the case of one output variable, but the generalization to several outputs is straightforward if the errors on each variable can be assumed independent. Observed outputs are denoted by  $\tilde{\mathbf{Q}} = (\tilde{q}_t)_{t=1, \dots, T}$ . Similarly, true and observed inputs are denoted by  $\mathbf{X} = (x_t)_{t=1, \dots, T}$  and  $\tilde{\mathbf{X}}$ . In this paper, a CRR model using evapotranspiration and rainfall as forcing data will be used. The evapotranspiration series will be assumed to be error-free. In order to simplify notation, the dependence of model output to evapotranspiration will be omitted thereafter, and  $\mathbf{X}$  will therefore simply denote rainfall.

True outputs are assumed to be corrupted by a Gaussian additive measurement error, whose variance  $\sigma_y^2$  is assumed to be known (1). The hypothesis of Gaussian errors with known variance is made for convenience in this paper, but the BATEA model can also be defined with alternative output error distributions with unknown parameters, whose inference is required.

$$y_t = \tilde{y}_t + \varepsilon_t, \quad \varepsilon_t \sim N(0; \sigma_y^2) \quad (1)$$

True rainfalls are assumed to be corrupted by multiplicative stochastic errors:

$$x_t = \tilde{x}_t \varphi_t, \quad \varphi_t \sim p(\varphi | \boldsymbol{\alpha}) \quad (2)$$

Following the framework proposed by Kavetski *et al.* (2006a, 2006b), rainfall errors are therefore treated as latent variables  $\varphi_t$ , sampled from the hyperdistribution  $p(\varphi | \boldsymbol{\alpha})$  with unknown hyperparameter vector  $\boldsymbol{\alpha}$ . The multiplicative nature of rainfall errors has been assumed by several authors (Kavetski *et al.*, 2006a, Oudin *et al.*, 2006, Ajami *et al.*, 2007) and seems to be a reasonable hypothesis, but it does not allow the handling of errors affecting zero-measured rainfalls. However, alternative input error models could be considered within the BATEA framework.

The CRR model is represented as a function  $h$  that maps the true forcing  $x_t$  into the true response  $q_t$  depending on a set of  $N$  parameters  $\boldsymbol{\omega}$ :

$$q_t = h(\mathbf{x}_{1:t}, \boldsymbol{\omega}) \quad (3)$$

Conceptualizing the catchment behaviour in a lumped way implies using temporally and spatially averaged quantities, which prevents the spatial and temporal variability of hydrological phenomena to be accounted for. Consequently, even if the true input/output data were known, the CRR model would not be able to exactly reproduce the true runoff, whatever the parameter values used. Kuczera *et al.* (2006) therefore proposed to explicitly recognize the stochastic nature of CRR models, by means of stochastic parameters. The CRR parameter set is thus partitioned into  $\boldsymbol{\theta} = (\boldsymbol{\theta}^{(1)}, \dots, \boldsymbol{\theta}^{(N_s)})$ , the set of stochastic parameters, and  $\boldsymbol{\omega} = (\omega^{(1)}, \dots, \omega^{(N_D)})$ , the set of deterministic parameters, with  $N_s + N_D = N$ . The  $i^{\text{th}}$  stochastic parameter at time step  $t$  therefore takes the following value:

$$\theta_t^{(i)} \sim p(\theta^{(i)} | \boldsymbol{\beta}^{(i)}) \quad (4)$$

As with rainfall errors, stochastic parameters are handled by means of latent variables  $\theta_t^{(i)}$ , with given hyperdistribution  $p(\theta^{(i)} | \beta^{(i)})$  and unknown hyperparameters  $\beta^{(i)}$ . The notation without superscripts  $\theta$  and  $\beta$  will be used hereafter to denote latent variables and hyperparameters of all stochastic CRR parameters.

The notation used here suggests that one latent variable is defined at each time step for parameters treated as stochastic and rainfall errors. However, it will be beneficial to reduce the dimension of the model by adding additional constraints on the temporal structure of latent variables. Up to now, all BATEA applications have been based on latent variables defined on a storm epoch time scale (Kavetski *et al.*, 2006a, b, Kuczera *et al.*, 2006). A storm epoch is defined as beginning with a rainfall exceeding a given threshold and ending with a dry spell exceeding a given duration. All rainfalls belonging to the same epoch are then assumed to be corrupted by the same multiplier. In this way, a unique latent variable is defined for each epoch. Similarly, stochastic parameters are assumed to be invariant within a storm epoch.

One of the objectives of this paper is to evaluate the sensitivity of BATEA estimates to the storm epoch hypothesis. An alternative temporal structure is therefore investigated for latent variables related to rainfall errors. Rainfall multipliers are assumed to affect a unique time step rather than a full epoch. In order to reduce the dimensionality of the model, a preliminary analysis is performed in order to evaluate which rainfalls are the most important to be corrected. Briefly, this analysis is based on the simulation of runoff series with corrupted inputs, whose errors are randomly sampled from a given distribution representing our prior belief about the possible range of errors. Only errors leading to a significant difference in simulated runoffs will be accounted for in the BATEA model, by defining a latent variable at this time step. Conversely, if errors affecting rainfall at time step  $t$  result in minor differences in simulated runoffs, this rainfall will be assumed to be error free, and no latent variable will be assigned for this time step.

## 2.2. Posterior distribution

The BATEA objective is to infer all parameters of the model, that is:

- Deterministic CRR parameters  $\omega$
- Latent variables of stochastic CRR parameters  $\theta^{(i)}$ ,  $i=1, \dots, N_S$
- Hyperparameters of stochastic CRR parameters  $\beta^{(i)}$ ,  $i=1, \dots, N_S$

- Latent variables of rainfall errors  $\varphi$
- Hyperparameters of rainfall errors  $\alpha$

Following Bayes' rule, the posterior pdf of these parameters can be derived as follows:

$$p(\omega, \theta, \beta, \varphi, \alpha | \tilde{Q}, \tilde{X}) \propto p(\tilde{Q} | \omega, \theta, \beta, \varphi, \alpha, \tilde{X}) p(\omega, \theta, \beta, \varphi, \alpha | \tilde{X}) \quad (5)$$

Let us first consider the likelihood of observed outputs. Using the output error model (1), we can write:

$$p(\tilde{Q} | \omega, \theta, \beta, \varphi, \alpha, \tilde{X}) = \prod_{t=1}^T N(\tilde{q}_t | q_t; \sigma_y^2) \quad (6)$$

The true output  $q_t$  is here unobserved, but will be modelled using true inputs of the hydrological model:

$$q_t = h(\mathbf{x}_{1:t}, \omega, \theta_{1:t}) \quad (7)$$

True inputs are also unobserved, but using error model (2), the following equation can be derived:

$$q_t = h(\varphi_{1:t}, \tilde{\mathbf{x}}_{1:t}, \omega, \theta_{1:t}) \quad (8)$$

This equation shows that the likelihood of observed outputs does not depend on any hyperparameters, but only on deterministic CRR parameters and latent variables of rainfall errors and stochastic parameters. Hence we have

$$p(\tilde{Q} | \omega, \theta, \beta, \varphi, \alpha, \tilde{X}) = p(\tilde{Q} | \omega, \theta, \varphi, \tilde{X}) = \prod_{t=1}^T N(\tilde{q}_t | h(\varphi_{1:t}, \tilde{\mathbf{x}}_{1:t}, \omega, \theta_{1:t}); \sigma_y^2) \quad (9)$$

The prior distribution of parameters can be decomposed as follows:

$$\begin{aligned} p(\omega, \theta, \beta, \varphi, \alpha | \tilde{X}) &= p(\omega, \theta, \beta, \varphi, \alpha) \\ &= p(\theta, \varphi | \omega, \beta, \alpha) p(\omega, \beta, \alpha) \\ &= p(\theta | \omega, \beta, \alpha) p(\varphi | \omega, \beta, \alpha) p(\omega, \beta, \alpha) \\ &= p(\theta | \beta) p(\varphi | \alpha) p(\omega) p(\beta) p(\alpha) \end{aligned} \quad (10)$$

Several assumptions have been made deriving this equation. First, the prior distribution specification does not depend on observed inputs (first line). Second, conditionally to the hyperparameters and deterministic parameters, latent variables describing rainfall errors and stochastic CRR parameters are mutually independent (third line). Last, the prior distributions of hyperparameters

and deterministic parameters are mutually independent (last line)

Merging equations (9) and (10) finally leads to the following expression for the posterior distribution:

$$p(\omega, \theta, \beta, \varphi, \alpha | \tilde{Q}, \tilde{X}) \propto p(\tilde{Q} | \omega, \theta, \varphi, \tilde{X}) \times p(\theta | \beta) p(\varphi | \alpha) p(\omega) p(\beta) p(\alpha) \quad (11)$$

The posterior derived from this hierarchical model is therefore made up of three parts (up to a constant of proportionality): likelihood of observed outputs, hyper-likelihoods of latent variables and priors of deterministic parameters and hyperparameters. Exploration of such a high-dimensional function is computationally challenging but not infeasible. Specific strategies for optimization and MCMC sampling are described in details by Kavetski *et al.* (2006c, 2006d, 2007) and Kuczera *et al.* (2007).

### 3. SYNTHETIC CASE STUDY

#### 3.1. Data

Time series of 366 daily rainfall and potential evapotranspiration (*pet*) for the Abercrombie catchment (with area 2770 km<sup>2</sup>) were used. These series will be considered as the ‘true’ input data. The logSPM CRR model (Kuczera *et al.*, 2006) was used to simulate daily streamflow discharge. Three sets of synthetic input/output data were generated, whose properties are summarized in Table 1:

D1.a: ‘True’ output runoff data were simulated using the true inputs and LogSPM model with parameters values shown in Table 2. Observed runoff was derived by corrupting the true output with an additive white noise generated from a  $N(0, 0.05^2)$  distribution. Observed rainfall was derived by multiplying each non-zero rainfall by  $1/\varphi_t$ , with  $\log(\varphi_t) \sim N(-0.2, 0.2^2)$ . Observed *pet* series remained identical to the true one.

D1.b: True and observed output were identical to the ones derived in D1.a data set. Observed rainfall was derived by multiplying all rainfall within a same storm epoch by an identical multiplier  $1/\varphi_t$ ,  $\log(\varphi_t) \sim N(-0.2, 0.2^2)$ . Storm epochs were defined by inter-epochs dry spells of at least two days, and starting rainfall of at least 0.5 mm. 37 such epochs were identified during the 366 days used for calibration.

D2: ‘True’ output runoff data were simulated using the true inputs and LogSPM model with parameter values shown in Table 2, except parameter *sK*, which is treated as stochastic with its log-transformed value randomly sampled from  $N(-2.3, 0.2^2)$  at the beginning of each storm epoch. Observed runoff was derived by adding white noise generated from  $N(0, 0.05^2)$ . Observed rainfall was derived by multiplying each non-zero rainfall by  $1/\varphi_t$ , with  $\log(\varphi_t) \sim N(-0.2, 0.2^2)$ .

**Table 2.** Parameter values used to generate synthetic data.

Number	Name	Value
1	sK	exp(-2.3)
2	sF	exp(7.8)
3	ssfMax	exp(4.6) mm/day
4	rgeMax	exp(3) mm/day
5	kBf	exp(-9)
6	kStream	exp(-0.75)
7	initSoil	30 mm
8	initGw	1000 mm
9	initStream	0.1 mm

#### 3.2. Sensitivity to input error hypotheses

In this section, the robustness of BATEA estimates in the presence of misspecification of rainfall error model is evaluated. Two different types of misspecifications are investigated: distribution misspecification (e.g. the hyperdistribution used in BATEA is Gaussian whereas the true input errors are log-normally distributed) and temporal structure misspecification (e.g. latent variables

**Table 1.** Synthetic data sets properties

Data set	D1.a	D1.b	D2
Description	Daily rainfall errors	Epoch rainfall errors	Daily rainfall errors + model errors
True input	<i>r</i> and <i>pet</i> from Abercrombie catchment		
Observed input	$\tilde{r}_t = r_t / \varphi_t$ $\tilde{p}et = pet$	$\tilde{r}_t = r_t / \varphi_{epoch(t)}$ $\tilde{p}et = pet$	$\tilde{r}_t = r_t / \varphi_t$ $\tilde{p}et = pet$
True output	Simulated from logSPM with fixed parameters		Simulated from logSPM with epoch stochastic parameter <i>sK</i> $\log(sK_{epoch(t)}) \sim N(-2.3, 0.2^2)$
Observed output	$\tilde{q}_t = q_t + \varepsilon_t, \varepsilon_t \sim N(0, 0.05^2)$		

defined on a storm epoch basis, whereas inputs are corrupted by daily errors). Six BATEA models are therefore fitted to the data D1.a and D1.b. All six models involve the estimation of four deterministic CRR parameters (Table 3) with the two remaining CRR parameters fixed at their true value to avoid numerical difficulties due to strong parameter dependence. The six BATEA models differ by the hypotheses used to define latent variables and the related hyperdistribution. Two temporal structures and three hyperdistributions are investigated as follows:

**Temporal structures:** The latent variables are defined either on a storm epoch basis or on a daily basis. In the storm epoch case, the storm definition is identical to the one used for deriving the data set D1.b. In the daily case, only the most informative daily latent variables have been included in the model, as explained in section 2.1.

**Hyperdistributions:** For each of these temporal structures, three hyperdistributions are used to model rainfall errors: a normal, a log-normal and a mixture distribution. Table 4 describes these

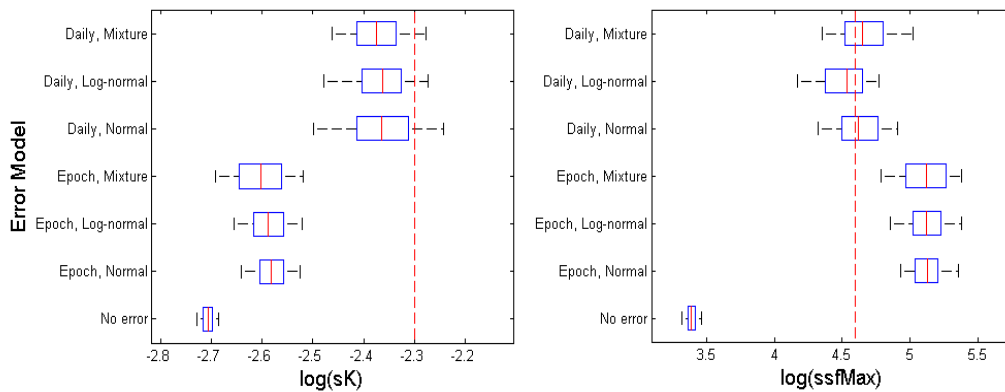
distributions, together with assumed priors of hyperparameters.

**Table 3.** Prior distributions of CRR parameters

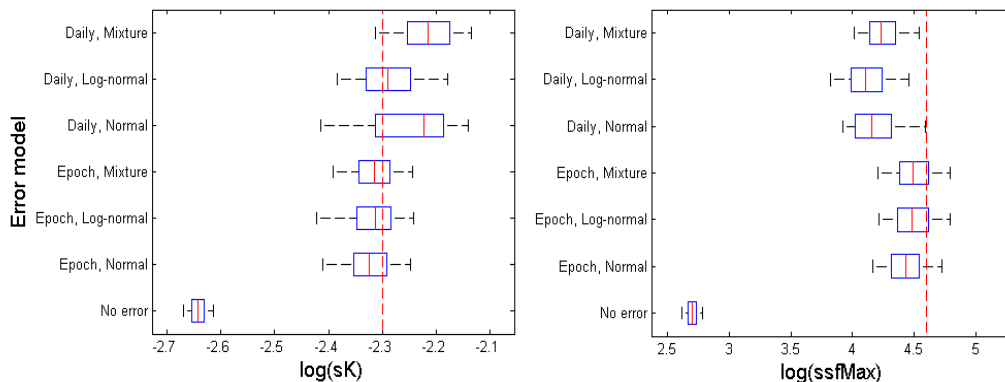
Parameter	Prior distribution
$sK$	$\log(sK) \sim N(-2; 2^2)$
$ssfMax$	$\log(ssfMax) \sim N(1; 2^2)$
$kBf$	$\log(kBf) \sim N(-6; 3^2)$
$kStream$	$\log(kStream) \sim N(-1; 2^2)$

In addition to these six models, a model assuming no input errors has been used to evaluate the influence of these errors on parameters estimates. Such a model is similar to a standard least squares (SLS) estimation.

These seven models were applied to the D1.a data, and the posterior distribution was explored using the MCMC strategy outlined in Kuczera *et al.* (2007). The marginal posterior distributions of two estimated CRR parameters are shown in Figure 2 as boxplots, whose boxes extend from the first to the third quartile and whiskers extend between 0.05 and 0.95 quantiles. Only results related to



**Figure 2.** Marginal posterior distributions of two inferred CRR parameters, with seven BATEA models. Rainfall is corrupted by daily errors.



**Figure 3.** Marginal posterior distributions of two inferred CRR parameters, with seven BATEA models. Rainfall is corrupted by epoch errors.

parameters  $sK$  and  $ssfMax$  are shown for conciseness, but results obtained for  $kBf$  and  $kStream$  are similar. The first observation is that ignoring input data errors leads to strong biases in parameter estimates. Biases also appear when assuming epoch errors when in fact daily errors corrupt input data. Conversely, no significant bias is observed when using daily latent variables for modelling rainfall errors, whatever the hyperdistribution. Moreover, within a given temporal structure, results obtained with different hyperdistributions are very close. These results suggest that parameter estimates are more sensitive to the temporal structure of latent variables than to the choice of hyperdistribution.

Results shown in Figure 3 were obtained using the D1.b data, whose rainfalls are corrupted by epoch errors. Once again, ignoring these errors leads to strong biases in the parameter estimates. The estimates obtained with models assuming epoch errors are unbiased. When assuming daily errors instead of true epoch errors, moderate bias occurs for parameter  $ssfMax$ , but this is clearly smaller than the biases previously observed when assuming epoch errors with daily corrupted data. Consequently, a model assuming daily errors seems to be more robust to temporal structure misspecification than a model using epoch latent variables. The impact of hyperdistribution misspecification seems to be of secondary importance with regard to parameter estimates.

### 3.3. Sensitivity to model error hypotheses

The robustness of BATEA estimates when model structural errors are misspecified is evaluated in this section. Synthetic data D2, including both input and model errors, are used for this purpose. Input errors are assumed to follow a log-normal distribution, and related latent variables are defined on a daily basis. Model errors are handled by considering  $sK$  parameter as stochastic, with log-normal hyperdistribution and latent variables defined on a storm epoch basis. Four different BATEA models are therefore considered, differing by the rules used to define the storm epochs. The first model uses the same rules as those used to generate the synthetic data set, leading to 39 storm

epochs. This number is not strictly equal to the number of epochs derived for synthetic data generation (37) because the epochs' definition rules are here applied on corrupted input data. However, the model is very close to the synthetic truth, and will therefore be considered as adequately specified. Three additional BATEA models are obtained by increasing the rain threshold used to define epochs, resulting in the number of epochs decreasing in the sequence 27, 19 and 11. The temporal resolution of model errors is therefore progressively altered in BATEA, thus increasing the misspecification of model errors.

BATEA results for misspecified epoch are shown in Figure 1. The first observation is that BATEA is able to discriminate model and input errors, as their hyperparameters are adequately estimated with a temporal resolution of 39 epochs. When this temporal resolution decreases, biases appear for parameters  $ssfMax$  and  $kStream$ , but they remain moderate. Parameter  $kBf$ , which controls the production of baseflow, seems to be more robust to model error misspecification. Surprisingly, the hyperparameters of the stochastic parameter  $sk$  are acceptably estimated, despite the misspecifications affecting the latent variables related to this parameter. This can be explained by considering estimated hyperparameters of input errors: although the hyper-mean is free from any bias whatever the temporal resolution, the hyper-standard deviation increases when the number of epochs decreases, leading to a significant overestimation of the true standard deviation of rainfall multipliers. This means that input errors compensate for model errors, because the number of latent variables for stochastic parameter  $sK$  is not sufficient to describe its variability.

Such a compensation mechanism has both advantages and drawbacks. The primary benefit is that it allows the bias in parameter estimates to remain moderate, despite an inadequate specification of model errors. Such robustness is an important feature in a regionalisation perspective, because not all structural errors can be accounted for by simply treating some parameters as stochastic. It is therefore anticipated that input errors will have to compensate for non-modelled

**Table 4.** Probability models used for latent variables describing rainfall errors

Hyperdistribution	Probability model	Prior distribution
Normal	$\varphi_i \sim N(\mu, \sigma^2)$	$\mu \sim U[0.5; 1.5]$ ; $\sigma^2 \sim U[10^{-5}; 1]$
Log-normal	$\log(\varphi_i) \sim N(\mu, \sigma^2)$	$\mu \sim U[\log(0.5); \log(1.5)]$ ; $\sigma^2 \sim U[10^{-5}; 1]$
Mixture	$\log(\varphi_i) \sim pN(\mu, \sigma_1^2) + (1-p)N(\mu, \sigma_2^2)$ ( $\sigma_1 \leq \sigma_2$ )	$p \sim U[0; 1]$ ; $\mu \sim U[\log(0.5); \log(1.5)]$ $\sigma_1^2 \sim U[10^{-5}; 1]$ ; $\sigma_2^2 \sim U[10^{-5}; 1]$

structural errors in real-world case studies. The primary drawback is related to the interpretation of estimated input errors characteristics: what is identified as input errors by BATEA might not only be rainfall measurement errors, but might also encompass a part of model structural error.

#### 4. CONCLUSION

This paper aimed at evaluating the sensitivity of CRR parameter estimates to the choice of error models. Several conclusions can be drawn from this study. First, parameter estimates are more sensitive to the temporal structure used to model input errors than to the chosen hyperdistribution. Second, using latent variables of rainfall errors defined on a daily basis leads to more robust estimates than the storm epoch-based definition of latent variables. Lastly, parameter estimates were found to be reasonably robust facing structural error misspecification. This robustness is achieved thanks to an artificial increase of input error variance, which compensates for unaccounted structural errors.

In this paper, the focus was on CRR parameters estimation. However, a similar study could be undertaken to evaluate the robustness of predictive uncertainty quantification in the presence of error model misspecification. One would expect predictive uncertainty to be more sensitive to hyperdistribution or structural error model misspecification.

#### 5. ACKNOWLEDGEMENTS

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