A Bayesian alternative for multi-objective ecohydrological model specification

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Abstract
Recent studies have identified the importance of vegetation processes in terrestrial hydrologic systems. Process-based ecohydrological models combine hydrological, physical, biochemical and ecological processes of the catchments, and as such are generally more complex and parametric than conceptual hydrological models. Thus, appropriate calibration objectives and model uncertainty analysis are essential for ecohydrological modeling. In recent years, Bayesian inference has become one of the most popular tools for quantifying the uncertainties in hydrological modeling with the development of Markov chain Monte Carlo (MCMC) techniques. The Bayesian approach offers an appealing alternative to traditional multi-objective hydrologic model calibrations by defining proper prior distributions that can be considered analogous to the ad-hoc weighting often prescribed in multi-objective calibration. Our study aims to develop appropriate prior distributions and likelihood functions that minimize the model uncertainties and bias within a Bayesian ecohydrological modeling framework based on a traditional Pareto-based model calibration technique. In our study, a Pareto-based multi-objective optimization and a formal Bayesian framework are implemented in a conceptual ecohydrological model that combines a hydrological model (HYMOD) and a modified Bucket Grassland Model (BGM). Simulations focused on one objective (streamflow/LAI) and multiple objectives (streamflow and LAI) with different emphasis defined via the prior distribution of the model error parameters. Results show more reliable outputs for both predicted streamflow and LAI using Bayesian multi-objective calibration with specified prior distributions for error parameters based on results from the Pareto front in the ecohydrological modeling. The methodology implemented here provides insight into the usefulness of multiobjective Bayesian calibration for ecohydrologic systems and the importance of appropriate prior distributions in such approaches.

1. Introduction

In recent years, the interaction between water resources and ecosystems has become a central topic among scientists because of the important role of vegetation dynamics in the catchment water cycle (Porporato et al., 2002; Asbjornsen et al., 2011). On one hand, water controls vegetation growth, photosynthesis, respiration and nutrient cycling. On the other hand, vegetation influences the water cycle through biochemical and biophysical processes such as evapotranspiration and rainfall interception (Chen et al., 2014). Ecohydrology integrates catchment hydrological and ecological processes and provides a framework within which the complex interrelationship between vegetation dynamics and water flows can be well investigated (Asbjornsen et al., 2011). The continuous dynamic models that combine conceptual and physical descriptions of hydrological, physical and biogeochemical processes such as water, heat, carbon and energy transmission are called process-based ecohydrological models. Commonly used model structures across scientific research and application include well-known models such as SWAT (Arnold et al., 1993; Arnold et al., 1998), SWIM (Krysanova et al., 1998; Krysanova et al., 2000), RHESSys (Band et al., 1993; Tague and Band, 2004), and Tethys-Chloris (Fatichi et al., 2012). Conceptual ecohydrological models are also widely used because of their model parsimony which makes it easier for model calibration (Istanbulluoglu et al., 2012; Viola et al., 2014). Due to the development of Geographical Information Systems (GIS) and remote sensing technology, studies of ecohydrological models have accelerated. However, describing the interactions between hydrologic and ecologic systems requires increasing model dimensionality and data for model conditioning. As a result, appropriate calibration objectives and model

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uncertainty analysis are essential for ecohydrological modeling. Ecohydrological model inference is also made more challenging by the need to represent the dynamics of multiple catchment state variables including streamflow and biomass production. Thus, there is a need for approaches to parameter specification that capitalize on all information that may be available to describe catchment scale ecohydrologic processes.

In recent years, multi-objective model optimization has emerged as a popular tool across multiple disciplines to derive parameter estimates that reproduce multiple model criteria or types of system observations. Multi-objective model calibrations are a common tool in model optimization of environmental systems. These approaches are frequently used when the objectives are under circumstances such that there are in conflicts with each other (Konak et al., 2006). The benefit of multi-objective optimization is that it provides a set of possible solutions which satisfies all the objectives in an acceptable range based on the concept of trade-offs. (Yapo et al., 1998). The output of this approach is a set of solutions which cannot be improved in each of the objectives without deteriorating the other. These solutions are usually called non-dominated, non-inferior or Pareto solutions (Elstratidis and Koutsoyiannis, 2010). Based on this concept, many multi-objective algorithms have been developed, including the Multi-Objective Genetic Algorithm (MOGA) ( Fonseca and Fleming, 1993), the Nondominated Sorting Genetic Algorithm (NSGA) (Srinivas and Deb, 1994), the Multi-objective Complex Evolution (MOCOM) (Yapo et al., 1998) algorithm, the Multi-objective Shuffled Complex Evolution Metropolis algorithm (MOSECM) (Vrugt et al., 2003a) and the Multi-algorithm, genetically adaptive multi-objective (AMALGAM) (Vrugt and Robinson, 2007) method. Note that individual objectives may represent different statistical summaries of a set of observations, or observations of different variables within the system being studied. In hydrological studies, one example may be when considering the trade-offs of the parameterization between high flows and low flows (Madsen, 2000; Shafii and Smelt, 2009).

In ecohydrological modeling (where typically an ecological sub-model is combined with a hydrological component), the optimization of the objective describing the ecological component may not be acceptable for the hydrological component, and vice versa. The benefits of using a multi-objective approach in an ecohydrological model (where we consider the interrelationship between the hydrologic cycle and vegetation dynamics) are obvious, as it provides a formal way in which to simultaneously and comprehensively consider both hydrological and ecological components of the model. Therefore, multi-objective optimization approaches are well suited to ecohydrological models. For instance, Naseem et al. (2015) presented a work of multi-response optimization for two conceptual ecohydrological models across 27 catchments in Australia. Results showed that the multi-objective optimization provided a better representation of the two response outputs (streamflow and leaf area index (LAI)) and has the potential to greatly improve ecohydrological modeling and applications.

While these multi-objective optimization approaches are useful for estimating deterministic parameter values that provide appropriate fits to competing calibration objectives, Pareto-based multi-objective calibration does not provide probabilistic solutions for the model parameters or any uncertainty analysis of the corresponding model predictions (Reichert and Schuwirth, 2012). With the development of Markov chain Monte Carlo (MCMC) methods and advances in computing power, Bayesian inference has emerged as a popular tool for uncertainty analysis in hydrological modeling (e.g. Bates and Campbell, 2001; Kuczera, 1983; Marshall et al., 2004; Smith and Marshall, 2008; Vrugt et al., 2003b). Bayesian inference provides a framework within which prior information and the data can be combined. It allows the statistical quantification of model uncertainties.

Compared with purely conceptual rainfall–runoff models, it can be argued that ecohydrological models may be more susceptible to uncertainty. One reason is that process-based models usually contain physically based mathematical descriptions as well as conceptual components. The complexity of model leads to possibly large model uncertainty (Arnold et al., 2009). Another reason is that often in ecohydrologic modeling different sources and sampling methods are used to collect catchment data, leading to multiple potential sources of observational uncertainty that influence model predictions and reliability. For example, in our case Leaf Area Index (LAI) data at an 8-day 1 km resolution via MODIS (Moderate Resolution Imaging Spectroradiometer) are used for calibration of an ecohydrologic model to capture vegetation dynamics. Compared with daily stream flow data, this LAI data likely contains more uncertainties (or less information) because of the coarse resolution and the error from the model that LAI is derived from. In lumped conceptual ecohydrological models another sources of uncertainty in LAI are related to the aggregation of LAI pixels inside a catchment to obtain mean catchment scale LAI. Therefore, the potential errors associated with LAI and streamflow observations would not be the same—that is, the two objective functions should not be equally weighted in an optimization problem. It is thus important to appropriately define the objective functions weights in a way that reflect the confidence level of observations. More recently, multi-objective Bayesian inference has been proposed as an alternative to traditional Pareto based multi-objective optimizations (Minet et al., 2015; Sikorska et al., 2015; Reichert and Schuwirth, 2012). These approaches are appealing as they allow model conditioning with multiple data sources, and provide a framework in which prior information can be used as a surrogate for traditional weighting of different model objectives.

In this study, we implement a multi-objective Bayesian calibration for a conceptual ecohydrologic model and demonstrate the usefulness of such an approach for inferring multiple catchment variables. We aim to develop appropriate prior distributions and likelihood functions that minimize model uncertainties within the framework based on information obtained from Pareto-based multi-objective optimization. The overall goal of this study is to combine traditional multi-objective calibration of ecohydrologic models with more recent Bayesian approaches, and demonstrate how an understanding of the Pareto front can help inform Bayesian calibrations.

2. Bayesian multi-objective inference

Multi-objective optimization aims to provide a set of possible solutions in front of the modelers. However, it doesn't provide probabilistic solutions. In our study, we aim to find an alternative for Pareto-based multi-objective optimization for an ecohydrologic model. A Bayesian multi-objective framework is presented considering different emphasis (via the prior distribution) on each objective. Reichert and Schuwirth (2012) introduced a method combining prior knowledge and multi-objective calibration. The preferred weight of each objective can be defined in the prior of error parameters. The prior of error parameters are defined as zero mean and favoring narrow distribution over wider distribution for one objective when the modeler wants to put more weight on it. Such an approach holds promise among mapping studies that attempt to infer multiple catchment or environmental variables. Recently, Sikorska et al. (2015) showed a comparison between Bayesian single and equal weighted multi-objective
calibrations in a combination of a rainfall-runoff model and a Total Suspended Solids (TSS) model. Minet et al. (2015) presented a case study of Bayesian multi-objective inversion in a dynamic vegetation model with different types of likelihood functions and prior information of the error parameters. These studies indicate the potential importance and application of multi-objective calibration in the ecohydrological modeling.

A conceptual ecohydrological model can be expressed as:

\[ O_t = f(x_t; \theta) + \epsilon_t \]

where \( O_t \) are the observations for a catchment at time \( t \), \( x_t \) is model inputs at time \( t \), \( \theta \) is the model parameter set, \( f(x_t; \theta) \) is the corresponding model output for time \( t \) and \( \epsilon_t \) is an error term.

In model specification via Bayesian inference, the posterior distributions of model parameters are estimated via Bayes’ theorem:

\[ P(\theta|O) = \frac{P(O|\theta)P(\theta)}{P(O)} \]

where \( P(\theta) \) is the prior distribution, which summarized the existing knowledge of the model parameters through parametric probability distributions, \( P(O|\theta) \) is the likelihood function which summarizes the model for the data given parameters, \( P(O) \) is a proportionality constant. The posterior distribution \( P(\theta|O) \) thus summarizes the parameter uncertainty after observing the data.

If the error term is assumed to be normally distributed, uncorrelated with constant variance \( \sigma^2 \), the log-likelihood function can be written as:

\[ L(O_t|\theta) = -\frac{N}{2} \log(2\pi \sigma^2) - \frac{1}{2 \sigma^2} \sum_{t=1}^{N} (O_t - f(x_t; \theta))^2 \]

Ecohydrological models simulate multiple variables that describe water, energy, and biophysical fluxes, such as streamflow, leaf area index (LAI), net primary production, and evapotranspiration. As such, the function presented here is extended so that \( O \) is a vector of observations at each time step. For a multivariate case, considering the error term follows multivariate Gaussian distribution:

\[ x \sim N(\mu, \Sigma) \]

Then the log-likelihood function can be expressed as:

\[ L(O_t|\theta) = -\frac{N}{2} \log(2\pi \Sigma) - \frac{1}{2} \sum_{t=1}^{N} (O_t - f(x_t; \theta))^T \Sigma^{-1} (O_t - f(x_t; \theta)) \]

Parameters being calibrated include model parameters and error parameters \( (\sigma^2_1 \text{ and } \sigma^2_2) \) for each of the objectives. The corresponding prior can be expressed as \( P(\theta), P(\sigma^2_1) \text{ and } P(\sigma^2_2) \). Hence, the log-posterior distribution can be expressed as:

\[ LP(\theta|O_t) = L(O_t|\theta) + LP(\sigma^2_1) + LP(\sigma^2_2) \]

3. Methodology

In our case studies, we aim to take advantage of traditional multi-objective calibrations to derive meaningful prior distributions for the Bayesian approach, and demonstrate how the Pareto front might be interpreted probabilistically. We first use the Multi-objective Shuffled Complex Evolution Metropolis (MOSCEM) algorithm (Vrugt et al., 2003a) to estimate possible parameter solutions along the Pareto front. Then, we calibrate the model using Bayesian multi-objective inference in different cases. Finally, we use the points on Pareto front to construct meaningful priors in the Bayesian framework, and the results are compared with the Pareto front.

3.1. Catchment and data

We selected Bloomfield River at China Camp (108003A), located in Daintree Basin, Queensland, Australia. The catchment area is 263 km² with an average annual rainfall of 2170 mm and average annual runoff of 1551 mm. Catchment elevation ranges between 151.2 m and 1272.5 m (http://www.ga.gov.au/elvis/) and 98% of its area is covered by trees (Lymburner et al., 2011). Daily Precipitation and PET data are from AWAP (Australian Water Availability Project), daily stream flow data is from HRS (Hydrologic Reference Stations, Australian Bureau of Meteorology), and 8-day LAI data from MODIS (Moderate Resolution Imaging Spectro radiometer). The LAI data are filtered at every pixel (1 km resolution) using the Svitisky-Golay method using the TIMESAT software (Jonsson and Eklundh, 2002, 2004). Then the catchment averaged values are calculated and used in the calibration. Simulated green LAI is compared with MODIS LAI. Data set from 2001 to 2005 are selected. The maximum LAI value is 5.8 (leaf area m²/green area m²).

3.2. Model

In our study, a HYdrological MODel (HYMOD) (Boyle, 2001; Wagener et al., 2001) and a bucket grassland model (BGM) (Istanbulluoglu et al., 2012) are coupled (Fig. 1). HYMOD is a lumped conceptual rainfall-runoff model with six parameters. In the model, a nonlinear soil moisture tank is connected to two series of tanks in parallel (quick flow tanks and a slow flow tanks) with different residence times. BGM is a vertically lumped bucket ecohydrological model which simulates biomass dynamics, and is coupled to the soil moisture tank in HYMOD. Modifications to the BGM are made based on formulation of Zhou et al. (2013) to simulate biomass growth in trees. We also replaced soil moisture dynamics in BGM with HYMOD soil moisture tank. Model inputs are daily precipitation and potential evapotranspiration. In the coupled model, the exchange terms between the two model components are ET and LAI. Soil moisture impacts ET by adjusting PET based on the available soil moisture, and ET controls net primary productivity (Eq. (3) in the Appendix) and subsequently biomass production (Eq. (5) in the Appendix). Estimated green biomass from the model is converted to LAI (Eq. (6) in the Appendix) which ultimately adjusts the input PET (Eq. (2) in Appendix). Adjusted PET with the intercepted rainfall influence the soil water balance. Model outputs are daily streamflow and LAI estimations. All the model parameters and the range values are listed in Table 1A. Seven parameters are being calibrated in the simulations which are marked as ‘Calibration’ in the last column in Table 1A. Model equations are described in the Appendix.

3.3. Bayesian multi-objective calibration

3.3.1. Multi-objective likelihood function

In the case study developed here, we calibrate our ecohydrologic model on observations of Leaf Area Index (LAI) and streamflow (Q) at different time steps. Assuming the error terms of each objective are independent, then the log multi-objective likelihood function can be expressed as:

\[ L_{\text{multi}} = L(Q|\theta) + L(LAI|\theta) \]

The type of error (i.e., homoscedastic or heteroscedastic error) was checked before this work using Smith et al. (2015)’s method. Tools such as residual scatterplot, quantile-quantile plot had been used to check the likelihood function for each of the objective. In our case study, the error term of streamflow (Q) is found to be
Gaussian, heteroscedastic and independent based on the test. Thus, the log likelihood is defined by applying the Box Cox transformation (Box and Cox, 1964):

\[
L(Q_t | \theta) = -\frac{N}{2} \log(2\pi) - \frac{N}{2} \log(\sigma_Q^2) - \frac{1}{2\sigma_Q} \sum_{t=1}^{N} (Q_t - f(x_t; \theta))^2 \\
- \log(Q_t + \lambda)
\]

where \( \lambda \) is the transformation parameter fixed at 0.3 based on Thyer et al. (2002)’s work for Queensland catchments in Australia. Similarly, the error term of LAI is Gaussian, homoscedastic and independent:

\[
L(LAI_t | \theta) = -\frac{N}{2} \log(2\pi) - \frac{N}{2} \log(\sigma_{LAI}^2) - \frac{1}{2 \sigma_{LAI}} \sum_{t=1}^{N} (LAI_t - f(x_t; \theta))^2 \\
- \log(Q_t + \lambda)
\]

So the log multi-objective likelihood becomes:

\[
L_{\text{multi}} = -N \log(2\pi) - \frac{N}{2} \log(\sigma_Q^2) - \frac{N}{2} \log(\sigma_{LAI}^2) \\
- \frac{1}{2 \sigma_Q} \sum_{t=1}^{N} (Q_t - f(x_t; \theta))^2 - \frac{1}{2 \sigma_{LAI}} \sum_{t=1}^{N} (LAI_t - f(x_t; \theta))^2 \\
- \log(Q_t + \lambda)
\]

3.3.2. Prior distributions

Traditional multi-objective optimization to estimate deterministic model parameters requires the modeler to specify a weighting on each objective that reflects the modeler’s belief in the importance of the objective or the reliability of the observations. In the Bayesian approach, this is implied via the specification of the prior distribution of the error variance parameters in the likelihood. The two error parameters \( \sigma_Q^2 \) and \( \sigma_{LAI}^2 \) in the likelihood function, reflect the “weight” of each objective to some extent (Reichert and Schuwirth, 2012; Minet et al., 2015). Therefore, the prior distributions for these variances should be defined carefully based on the modeler’s confidence level in the ecohydrologic observations. To see the influence of the prior distributions of error parameters, we define all the priors for the ecohydrologic model parameters as uniform distributions within the boundary value shown in

![Diagram](image-url)

**Fig. 1.** A conceptual rainfall-runoff model (HYMOD) and a dynamic vegetation model (DVM) are combined.

### Table 1A

<table>
<thead>
<tr>
<th>Parameters in HYMOD.</th>
<th>Description</th>
<th>Typical value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Huz</td>
<td>Height of soil moisture tank</td>
<td>0, Inf</td>
<td>Calibration</td>
</tr>
<tr>
<td>B</td>
<td>Distribution function shape</td>
<td>0, 2</td>
<td>Calibration</td>
</tr>
<tr>
<td>Alp</td>
<td>Quick-slow split</td>
<td>0, 1</td>
<td>Calibration</td>
</tr>
<tr>
<td>Nq</td>
<td>Number of quickflow tank</td>
<td>1, 4</td>
<td>Fix to Nq = 2</td>
</tr>
<tr>
<td>Kq</td>
<td>Quickflow routing rate</td>
<td>0, 1</td>
<td>Calibration</td>
</tr>
<tr>
<td>Ks</td>
<td>Slowflow routing rate</td>
<td>0, Kq</td>
<td>Calibration</td>
</tr>
</tbody>
</table>

### Table 1B

<table>
<thead>
<tr>
<th>Parameters in BGM.</th>
<th>Description</th>
<th>Typical value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Imax</td>
<td>Maximum daily interception (mm)</td>
<td>1</td>
<td>(1)</td>
</tr>
<tr>
<td>LAIref</td>
<td>LAI of reference crop</td>
<td>1.44</td>
<td>(2)</td>
</tr>
<tr>
<td>LAImax</td>
<td>Maximum live/green LAI</td>
<td>-</td>
<td>Catchment’</td>
</tr>
<tr>
<td>WUE</td>
<td>Water use efficiency (kg CO₂/kg H₂O)</td>
<td>0.001, 0.1</td>
<td>Calibration</td>
</tr>
<tr>
<td>w</td>
<td>Conversion factor (kg DM/kg CO₂)</td>
<td>0.55</td>
<td>(3)</td>
</tr>
<tr>
<td>mu</td>
<td>Ratio of night time to day time CO₂ net ecosystem exchange</td>
<td>0.3</td>
<td>(4)</td>
</tr>
<tr>
<td>SLAg</td>
<td>Specific leaf area for green biomass [m² leaf/g DM]</td>
<td>0.005</td>
<td>(5)</td>
</tr>
<tr>
<td>SLAd</td>
<td>Specific leaf area for dead biomass [m² leaf/g DM]</td>
<td>0.01</td>
<td>(5)</td>
</tr>
<tr>
<td>rb</td>
<td>Density of water (kg/m³)</td>
<td>999.9</td>
<td>–</td>
</tr>
<tr>
<td>PETmx</td>
<td>Constant for dead biomass loss adjustment (mm/day)</td>
<td>10</td>
<td>(5)</td>
</tr>
<tr>
<td>Ksg</td>
<td>Natural decay factor for live/green biomass (d⁻¹)</td>
<td>0.001, 0.02</td>
<td>Calibration</td>
</tr>
<tr>
<td>Ksr</td>
<td>Natural decay factor for live/green biomass (d⁻¹)</td>
<td>0.001, 0.02</td>
<td>Fix to 0.01</td>
</tr>
<tr>
<td>Kdd</td>
<td>Natural decay factor for live/green biomass (d⁻¹)</td>
<td>0.001, 0.02</td>
<td>Fix to 0.01</td>
</tr>
</tbody>
</table>

Source: (1) Scanlon and Albertson (2003); (2) Allen et al. (1989); (3) Scholes and Walker (2004); (4) Williams and Albertson (2004); (5) Istanbulluoglu et al. (2012).

* LAImax is fixed to 5.8 for the study catchment.

* DM: dry mass.
Then we define and compare three different types of prior distributions for the error parameters in the multi-objective calibration cases:

1. Multivariate uniform: both parameters \( \sigma^2_Q \) and \( \sigma^2_{LAI} \) are assumed uniformly distributed;
2. Multivariate weighted: \( \sigma^2_Q \) and \( \sigma^2_{LAI} \) are defined as normal distributions with mean of 0 truncated at zero and specified standard deviations, a smaller standard deviation is selected when more weight is emphasized on one of the objectives while a larger standard deviation is assigned to the less important objective;
3. Multivariate Pareto: \( \sigma^2_Q \) and \( \sigma^2_{LAI} \) are defined based on the results of the Pareto front estimated using an automatic multi-objective optimization.

In the first prior case, we consider the two objectives are effectively equally weighted, and we consider no a priori information available regarding our confidence in the catchment observations. The second prior case follows previous multi-objective work in environmental systems (Reichert and Schuwirth, 2012; Minet et al., 2015). The prior distributions are defined based on the principle that smaller errors are preferred and the difference of the standard deviation of the prior distributions reflect the preferred emphasis on each objective. In this case, a smaller standard deviation in one prior means more weight on this objective. The last prior case is based on the Pareto front output. From this approach, five different points on the Pareto front are randomly chosen and we consider this selection reflects the modelers’ different decisions of the ‘weight’ of each objective. We consider the prior in the last case as the most informative case as it forces increased error on the variables in which the modeler has less confidence regarding the validity of the model observations. We use Pareto front points to construct priors in Bayesian multi-objective calibrations with the aim of obtaining similar weights for each objective as the points on the Pareto front. As a result, these points will include probabilistic description of the model uncertainties in a Bayesian framework.

3.4. Calibrations setup

All calibration approaches and the methods used are listed in Fig. 2. For each simulation, the first 2 years of data were used as a warm-up or spin-up period to minimize the effect of initial condition assumptions regarding the initial LAI and catchment storage. For the Pareto-based multi-objective calibration, we use MOSCEM (Vrugt et al., 2003a) to optimize mean squared error (MSE) of Box cox transformed Q and MSE of LAI. MOSCEM method is the multi-objective expansion of the single objective optimization method SCEM-UA (Vrugt et al., 2003b). In the simulation, 10 complexes and 100 loops are defined.

For each of the Bayesian multi-objective calibrations, we employ the Adaptive Metropolis (AM) algorithm (Haario et al., 2001). For each simulation, 100,000 iterations are carried out – the first 10,000 iterations are discarded and the remaining 90,000 iterations are used to analyze the posterior distributions. Convergence is diagnosed via visualizing diagnostic plots of multiple MCMC runs to reduce computational demand (Marshall et al., 2004). To compare with the multi-objective calibrations, single objective calibrations on LAI or streamflow are also simulated using both the SCE-UA optimization (Vrugt et al., 2003b) and the Bayesian method.
4. Results

4.1. Single objective optimization

Firstly, single objective calibration of LAI and streamflow are performed using the SCE-UA method (Duan et al., 1994). The predicted and observed LAI and streamflow are plotted in Fig. 3. In each plot, the observed (red dots) and predicted LAI or Q (black and green lines) from both single objective calibrations are compared. It is obvious that for the variable type being optimized, simulations are improved and generally representative of the magnitude of the observations. However, the variable not being optimized is generally poorly simulated. This is particularly true for the case where LAI only is optimized. In this case, the simulated streamflow data are mostly close to zero for the recession period and small storm events can’t be captured.

4.2. Pareto front from multi-objective optimization

The Pareto front shows a clear tradeoff when either objective (stream flow or LAI) is optimized, generally reflecting the results of the individual variable optimizations (Fig. 4). From these results, five points are selected at specified intervals along the Pareto front representing different weighting applied to each variable. Based on these points, five sets of priors for error parameters are defined as normal distributions with means set at these values. In the multivariate uniform cases, variance of the prior distributions (5 and 0.1) are selected to represent different emphasis on each objective. In the multivariate Pareto cases, mean of the prior distributions are selected as the optimized MSE results from the five points on the Pareto front. Previous studies shown that the mean of the prior has more influence on the posterior than the variance of the prior (Tang et al., 2016). So here the variances of these priors are defined according to the order of magnitude of the Pareto front values. For transformed Q and LAI, 0.02 and 0.03 are selected respectively to keep the prior distributions at the same informative level and these variances remained the same for all these prior distributions. All the Bayesian simulations with different prior distributions are listed in Table 2.

The posterior distributions of the model parameters for different cases in Bayesian scenario are presented in Fig. 5. In this figure, the first two rows are the cases of single objective calibrations. The remaining six rows are the posteriors from the multi-objective cases using uniform prior and priors that are constructed based on the Pareto front (P1 to P5). In all the cases, the posterior distributions for five model parameters (three hydrology parameters and two vegetation parameters which are more important in the coupled processes) are shown in the first five columns and error parameters are shown in the last two columns in the figure. It can be seen that the posterior distributions in the LAI only case are all relatively diffuse, especially for the hydrologic parameters, suggesting that the hydrologic part of the model hasn’t been well calibrated in the LAI only case. It also can be seen that the model parameter posterior distributions from all the multi-objective cases are more similar to the streamflow only case compared to the LAI case, except for the distribution function shape parameter B which controls the shape of the catchment soil moisture storage. The posterior distributions of B in the multi-objective cases are closer to the estimation of the posterior from the LAI only case. Comparing the P1 to P5 cases, it is clear that the error parameter posteriors differ significantly depending on the assumed prior distribution. In addition, it is observed that the hydrologic model parameters don’t change significantly among the different cases, while vegetation parameters show clear differences.

4.3. Observed and predicted LAI data and stream flow data

We compare the predicted LAI and streamflow in multivariate weighted prior cases and uniform prior cases in Fig. 6. The Kullback-Leibler divergence (KLD) between the prior and posterior distributions of error parameters is calculated and shown in Table 3 following Tang et al. (2016). The KLD is a non-symmetric measure.
of the difference between two probability distributions. Variations in the KLD results can reflect the influence of the prior distributions on the posterior distributions. Less variations mean less impact of the prior on the posterior distributions, and large variations mean larger impact of the prior on the posterior. Comparing the changes of KLD among different cases, it is clear that the changes of KLD between the prior and posterior of error parameter LAI are significantly larger than Q (See the dramatic difference between constrained Q and constrained LAI cases for KLD LAI).

The predicted LAI from the constrained streamflow and uniform prior cases are very similar, showing similar streamflow and LAI magnitudes and dynamics. In contrast, the constrained LAI case differs considerably to the other cases and shows a simulation much closer to the observations. Predictions of streamflow from the three cases are all similar and, as expected, the predictions from constrained Q case are improved in comparison to the other two cases. The comparisons between observed and predicted LAI and stream flow data with 90% confidence limit in different cases are shown in Figs. 7 and 8. Confidence limits are calculated based on the variances of residual errors $\sigma_i^2$, so in the single objective calibration cases only the objective being calibrated has confidence limits included. Summary statistics of the computed confidence limit, the reliability and sharpness (Smith et al., 2015) are also included. The reliability is defined as the percentage of observations located in the 90% limit, and the sharpness is the mean of the width of the confidence limit. In each case a good result will mean that 90% of observations are captured by the 90% confidence limit in favor of narrower width.

Comparing the predicted LAI in the LAI only and multi-objective uniform cases in Fig. 7, the single LAI calibration case has much narrower confidence interval (mean width = 3.0344) than the multi-objective case (mean width = 4.7658), however, it is mildly overinflated (reliability 92.75%) compare to the multi-objective uniform case (reliability 89.13%). In the Pareto point based prior cases, P1 case has the best predicted LAI and P5 has the worst, as the P1 point is selected with better (smaller) LAI objective value than P5 on the Pareto front (Fig. 4). The differences of these statistics are less obvious for stream flow (Fig. 8). However, when comparing the five Pareto point cases, it is clear that the P1 case has the worst results compare to P5 case.

4.4. Pareto front vs. Bayesian outputs

The posterior distributions for the error parameters of the P1 to P5 cases are plotted as contours on the Pareto front (Fig. 9). The open circles shown here are the points on the Pareto front, and the five black dots represent the selected points used for defining

### Table 2

<table>
<thead>
<tr>
<th>Cases</th>
<th>Prior</th>
<th>(\sigma^2)</th>
<th>(\sigma_U)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single calibrations</td>
<td>Q only</td>
<td>(\sigma^2 \sim \text{Unif}(0.5))</td>
<td>(\sigma_U \sim \text{Unif}(0.5))</td>
</tr>
<tr>
<td></td>
<td>LAI only</td>
<td>(\sigma^2 \sim \text{Unif}(0.5))</td>
<td>(\sigma_U \sim \text{Unif}(0.5))</td>
</tr>
<tr>
<td>Multivariate Uniform</td>
<td>(1)</td>
<td>(\sigma^2 \sim \text{TN}(0.5))</td>
<td>(\sigma_U \sim \text{TN}(0.1))</td>
</tr>
<tr>
<td></td>
<td>(2)</td>
<td>(\sigma^2 \sim \text{TN}(0.01))</td>
<td>(\sigma_U \sim \text{TN}(0.5))</td>
</tr>
<tr>
<td>Multivariate Pareto</td>
<td>P1</td>
<td>(\sigma^2 \sim N(0.3546, 0.002))</td>
<td>(\sigma_U \sim N(0.7119, 0.003))</td>
</tr>
<tr>
<td></td>
<td>P2</td>
<td>(\sigma^2 \sim N(0.2487, 0.002))</td>
<td>(\sigma_U \sim N(0.7282, 0.003))</td>
</tr>
<tr>
<td></td>
<td>P3</td>
<td>(\sigma^2 \sim N(0.1895, 0.002))</td>
<td>(\sigma_U \sim N(0.7677, 0.003))</td>
</tr>
<tr>
<td></td>
<td>P4</td>
<td>(\sigma^2 \sim N(0.1777, 0.002))</td>
<td>(\sigma_U \sim N(0.8051, 0.003))</td>
</tr>
<tr>
<td></td>
<td>P5</td>
<td>(\sigma^2 \sim N(0.1619, 0.002))</td>
<td>(\sigma_U \sim N(1.0047, 0.003))</td>
</tr>
</tbody>
</table>

**Fig. 4.** Pareto front from MOSCEM optimization. The variance of the errors between measured and predicted streamflow (log-transformed, x-axis) is plotted against the variance of the errors between measured and predicted LAI (y-axis). Blue dots are the points on the Pareto front, and the dots in the pink boxes are randomly selected points that are used to define the prior distributions for error parameters in Bayesian calibrations. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
the prior distributions. The five groups of contours show the multivariate distributions of the error parameters from the Bayesian outputs. Agreement between Pareto solutions and Bayesian outputs can be seen from the figure. P2, P3 and P4 points all lie in the contour maps and close to the highest density, P1 and P5 points are relatively further away from the highest density but still lie in the multivariate distributions. The optimized values of the error parameters in (1) uniform prior, (2) constrained Q prior and (3) constrained LAI prior are also plotted as crosses in Fig. 9. The result for constrained LAI case located within the dominated space. Results from uniform case and constrained Q cases are very similar. The optimized LAI are much worse than the uniform case, but the optimized Q are similar in all these cases.

5. Discussion

5.1. Ecohydrological models and Bayesian multi-objective calibrations

Our study demonstrates the impact that available data has on the calibration process, and the difficulty in predicting catchment variables when only considering biomass or streamflow observations alone (Fig. 3). It is clear that optimized parameter values for the single objective calibration lead to poor simulations for the other variable that is not optimized. The poor simulation of LAI (green line) from the streamflow single objective calibration in Fig. 3(a) suggests that the calibrated parameter values from calibrating the hydrological component of the model are unable to represent the LAI dynamics. Therefore, a multi-objective optimization which simultaneously optimizes both objectives (LAI and Q) becomes necessary in an ecohydrological framework. However, in the meantime, more sources of uncertainties are involved in predicted outputs. To quantify model uncertainties and possibly further classify different sources of errors via a hierarchical approach a comprehensive Bayesian framework is essential. The Bayesian calibration is useful as it provides a clear analysis of the uncertainties in the model parameters. In a traditional calibration based on streamflow observations, there is no clear difference between the vegetation and streamflow parameters in terms of uncertainty as all parameters lie well within their prior distributions and boundaries. The Bayesian multi-objective approach

![Posterior distributions for model and error parameters from Bayesian calibrations. First five columns are the posterior for model parameters (Huz, B, Alp, Ksg, WUE) and the last two columns are the posterior for the model error parameters. Single objective calibrations (Q only/LAI only) are shown in the first two rows and the multi-objective calibrations using uniform prior and Pareto front information cases are shown in the last six rows (shown as Multi unif and P1 to P5).](image-url)
becomes more powerful when considering the differences between the parameters for different observation types (LAI or streamflow). The uncertainty in the parameters is highly dependent on the variables that are used to condition the models. For example, there are very different posterior distributions when streamflow is used to calibrate the model in comparison to LAI (Fig. 5, top panels). Streamflow has more information (posteriors are more peaked and narrower), even for calibrating the vegetation parameters (see, for example, the parameter WUE, Fig. 5 top panels). However, calibrating on LAI alone is still useful for providing informative parameter values as each parameter lies well within its a priori specified boundaries as mentioned in Table 1B (perhaps with the exception of the parameter Alpha). This has implications for the calibration of hydrologic models when streamflow observations are not available, as it suggests that LAI observations may be helpful to reduce uncertainty in the parameters of an ecohydrologic model, particularly for streamflow predictions in ungauged catchments.

5.2. Importance of prior distribution

According to the Bayesian rule, the posterior distribution is the prior distribution being updated given the available data sets. Generally, this means that the prior would have great influence on the posterior when data is limited, and with increased data length this impact will decrease. This leads to one important issue in the Bayesian related studies: how much information should the prior have. On one hand, in order to maintain objectivity it can be suggested that the prior should have little information or minimal impact on the data, and as such the non-informative prior is introduced (Jeffreys, 1946; Box and Tiao, 1973; Bernardo, 1979; Kass and Wasserman, 1996). On the other hand, when the data is limited or the parameter is insensitive to the data, an informative prior based on the experts’ knowledge or previous case studies should be used (Bates and Campbell, 2001; Freni and Mannina, 2010; Gharari et al., 2014; Hrachowitz et al., 2014). Recent research has considered the importance of the prior distribution as a function of the prior mean/variance and the length of data, and it is clear in some cases the prior can be strongly influential (Tang et al., 2016). Although there is no guidance in hydrologic related disciplines of when and how to specify meaningful priors, the study presented here a framework in which to formally incorporate prior information for multi-objective studies, by selecting different error parameter priors based on the results from the Pareto front in a multi-objective calibration problem. Results show that posterior distributions are strongly influenced by assuming different locations for the prior distributions of error parameters (Fig. 5). Comparing the posterior distributions among P1 to P5 cases with different prior distributions in Fig. 5, it can be observed that the hydrologic parameters remained similar among all the cases while the vegetation parameters varied considerably depending on different priors defined. In addition, the much larger differences of KLD for LAI error parameter among different cases than Q (Table 3) indicates that the error parameter LAI is much more sensitive to the prior than Q. Reasons for this could be either the LAI data has too little information or the vegetation parameters are very insensitive to the data. Therefore, a more meaningful and constrained prior should be defined for the vegetation parameters and more emphasis should be allocated on the calibration of LAI. This concept is similar as ‘limit of acceptability’ introduced by Blazkova and Beven (2009), which reflects the confidence level of the data and is defined before the simulations in their work. In our work, as there are more data used in the simulations, the amount of uncertainties for each data are suggested to be defined in the prior based on our knowledge of data. Another possible reason could be the function of the simple conceptual model structure for the vegetation dynamics. Further study should be considered on the investigation of the relative contribution of different uncertainty
sources (i.e., model structure uncertainty, input uncertainty) and the application for different ecohydrological models and catchments.

5.3. Defining appropriate weights for each objective

The selection of appropriate weights when calibrating to multiple objectives remains a point of interest in many automatic multi-objective calibration studies. There are two reasons that the objectives may not be just equally weighted in multi-objective calibrations. First of all, frequently sampling methods for obtaining the data being calibrated are different and thus the uncertainty in the data is not equal for different catchment variables. Secondly, the ‘information content’ in the data are not the same. The concept of ‘disinformation’ is introduced by Beven and Westerberg (2011). According to their work the information levels for data from different events are different. For multiple input data the variable carries more information will strongly influence the multi-objective calibrations. Therefore, the calibration ‘weights’ (which are defined in the prior of residual errors in the Bayesian approach) should be selected appropriately according to the reliability of each data being calibrated or based on the modeler’s preference of the accuracy level for the objectives.

The predicted LAI from constrained Q and uniform prior cases were very similar that the calibrations tended to optimize the streamflow rather than LAI, suggesting that the streamflow data has more information than LAI (Fig. 5). Similar evidence can be seen (Figs. 7 and 8) in that the predicted streamflow from uniform equal weighted multi-objective calibration was similar as the case calibrated on streamflow only. To balance the different information content in the data, it is suggested that more emphasis should be allocated to the observations which have less information. In our study, we defined the constrained LAI and constrained Q prior distributions to compare with the uniform prior case in the multi-objective calibration. The case using the constrained LAI case performed better than the other two cases where the predicted LAI was much closer to the observations and the predicted streamflow was not significantly worse than the multi uniform case at the same time (see Fig. 9, optimized estimation for weighted LAI, weighted Q and uniform cases are shown as red, green and blue

Fig. 7. 90% confidence limits of the residuals between measured and predicted LAI values from Bayesian calibration based on LAI only, the multi-objective case with uniform error priors and P1–P5 prior cases. A comparison of LAI from Q only case is shown in the last plot. In each plot the red dots are the measured LAI values and the black line is the predicted LAI, the confidence limit is shown in light blue shade. The computed statistics (reliability and the average width of the confidence band) are also shown on the right hand side of each plot. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
crosses) The error prior distributions used in this approach were defined according to Reichert and Schuwirth (2012)'s study.

In contrast to this, we implement here a new approach where we define a meaningful prior for the error parameters in a Bayesian multi-objective framework that represents the weights for each objective based on the results from the Pareto front. One of the benefits from the Pareto-based optimization is that the Pareto front perfectly shows the values of each objective given the selected weights, and as such can be a good reference in which to define the prior distribution in order to find the preferred weight in a Bayesian scenario. Comparing the computed statistics based on 90% confidence limits of the predicted LAI and streamflow from the cases using specified error prior distributions (Figs. 7 and 8, P1 to P5 cases), it can be clearly seen that in the P1 case (representing the prior with the largest implied emphasis on LAI and the least for streamflow) the predicted LAI was forced to fit the observation (and the corresponding sharpness was the smallest) while the simulated streamflow showed greater uncertainty (sharpness was the largest). In contrast, the P5 case (with least emphasis on LAI and most for streamflow) shows the narrowest confidence band for streamflow and widest band for LAI among all five cases. It suggests the fit of data (the weights for each objective) can be determined in the prior distributions. We then compared the Bayesian outputs with the Pareto front to see the level of agreement on each other.

5.4. Comparison between Pareto-based multi-objective optimization and Bayesian multi-objective calibration

Pareto-based multi-objective optimization aims to optimize all model objectives at the same time and to find a set of possible solutions that satisfy each of the objectives at an acceptable level. In our case the mean square error (MSE) of streamflow and LAI were simultaneously minimized (Fig. 4). Modelers can select any of the points on the Pareto front, and the process of the selection reflects the modelers’ preference or the weights of each objective. The outputs are a set of possible MSE combinations of each objective and the corresponding model parameter values. In contrast to this approach, in Bayesian multi-objective calibrations, the model log-likelihoods are maximized and the residual errors associated
with the model are sampled and updated, combing the prior distributions. The outputs are probability distributions of model parameters. In addition, there is no direct definition for the objective ‘weights’ or user preference in the formal Bayesian framework, this is implied through the prior distribution of the model and error parameters. Therefore, the results from Bayesian multi-objective calibration and Pareto-based optimization are not the same.

Pareto-based multi-objective optimization techniques have several great points to make them useful. It provides good consistency between objectives in terms of parameter optimizations and it allows modelers to choose the results they want to use in a set of optimal solutions. It is thus meaningful to combine Pareto optimization with formal Bayesian calibration, for utilizing all the information from Pareto solutions, and incorporating probabilistic

![Fig. 9](image_url) Multivariate contour plots (colored contours) of the posteriors of the error parameters from Pareto prior cases are plotted together with the Pareto front (black circles). Black dots represent the points selected for Pareto prior. Cross points are the optimal solutions of uniform prior case (blue), constrained Q case (green) and the constrained LAI case (red). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

![Fig. 10](image_url) A quality check of LAI observations is shown in the plot where the percentages of good quality LAI pixels over the entire catchment are calculated for each day. Red dots are the days that the percentages of good quality pixels are greater than 60% and the blue ones represent days when the percentages of good quality pixels are smaller than 60%. Black line is the simulated LAI from the LAI only case. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
analysis in the Bayesian framework. The results obtained from the Pareto-based optimization can be used to construct meaningful priors in the Bayesian framework. This approach is particular useful in a multi-objective calibration because it provides a mechanism by which to define meaningful prior distributions. Fig. 9 compares the Bayesian outputs (contours) and the Pareto front (circles) for the same case study. For each case (P1–P5), the Pareto front point used to define the prior distribution of the error variance lies within the error variance posterior distribution. This means that the calibrations are properly informed by the prior distributions representing the weights of each objective which are constructed based on the Pareto front. The agreement between these results demonstrates that our approach works well for simulating both LAI and streamflow outputs using the informative priors defined according to the weights selected on the Pareto front in the Bayesian multi-objective calibration framework. In addition, the probabilistic solutions from the Bayesian outputs summarizes the uncertainties for both objectives, making it possible for the further statistical analysis to be implemented.

5.5. Assessing reliability of model simulations

As the accuracy of simulated LAI are impacted by the quality of satellite observations, we performed several quality checks to validate the MODIS LAI observations. First, we confirmed that the MODIS landcover classification for the study catchment over the simulation period (2001–2005) are consistent and distribution of land cover types are consistent with Google Earth observations. Second, we used the MODIS LAI quality flags images for each day to assess the quality of reported LAI. Approximately 69% of all the LAI pixels within the catchment are classified as good quality data for the study period. The percentages of the good quality pixels for each day are shown in Fig. 10. In this plot, the red dots are the observations from the days that more than 60% of the pixels have good quality. The blue dots are the observations from the days when percentages of good quality pixels are less than 60%. The black line is the predicted LAI from LAI only case. It can be seen that the periods of the ‘off-tracked’ parts of simulated LAI (black line) always appear after the periods with bad quality LAI data (blue dots, where less than 60% of the pixels have good quality). This result demonstrates that the relatively poor calibration of LAI is at least partially due to the quality of LAI observations. Nevertheless, we would maintain that the LAI observations are captured by the uncertainty bands when LAI data are used to condition the model (Fig. 7). The uncertainty framework presented here highlights the potential tradeoffs when using a multi-objective approach. However, a detailed study that incorporates LAI uncertainty and assesses its impact on model simulations is inevitable in the future.

6. Conclusions

Bayesian multi-objective calibrations are compared with a Pareto-based multi-objective optimization using an ecohydrological model. Streamflow and LAI data are calibrated, making use of different prior distributions that might reflect the modelers’ degree of confidence in the system observations. Posterior distributions and confidence limits are compared for different case studies with different priors for error parameters: (1) same uniform priors; (2) constrained priors on the preferred objective; and (3) priors based on points on the Pareto front. From our results and analysis, we summarize the following conclusions and the possible future work:

- As ecohydrological models usually combine hydrological and ecological components in the model, it is recommended to apply multi-objective calibration to simultaneously optimize hydrological/ecological objectives.
- In a Bayesian framework, the preferred weights of each objective can be constrained by defining different priors for error parameters. However, it is hard to derive ‘true’ priors for each error parameters, as these must reflect the modelers a prior understanding of the uncertainty inherent in the model and the catchment observations. We have demonstrated here the selection of appropriate priors based on the Pareto front as a way to define informative priors and to bring a modelers understanding of classical multi-objective optimization to the Bayesian framework. Therefore, we recommend the use of this approach when a Bayesian multi-objective calibration is needed.
- The approach we presented is flexible and can be applied to a wide range of models. It can be used in the models when accurate estimation of more than one variable is desired. For instance, different variables such as ET, soil moisture and other biomass observations can be selected as objectives for ecohydrological modeling depending on the available data and calibration requirements. A Bayesian multi-objective calibration approach which has three likelihood functions with specified weights for each objective could be implemented combing many-objective optimization techniques such as Hurford et al. (2014)’s work.
- Future work will be further focused on the impact of different sources of uncertainties (such as input uncertainties), including defining proper error models and investigating the different impacts of uncertainties on each of objective.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.jhydrol.2017.07.040.

References
