MCMC-Bayesian Calibration of the Community Land Model for the US-ARM site

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OBJECTIVE

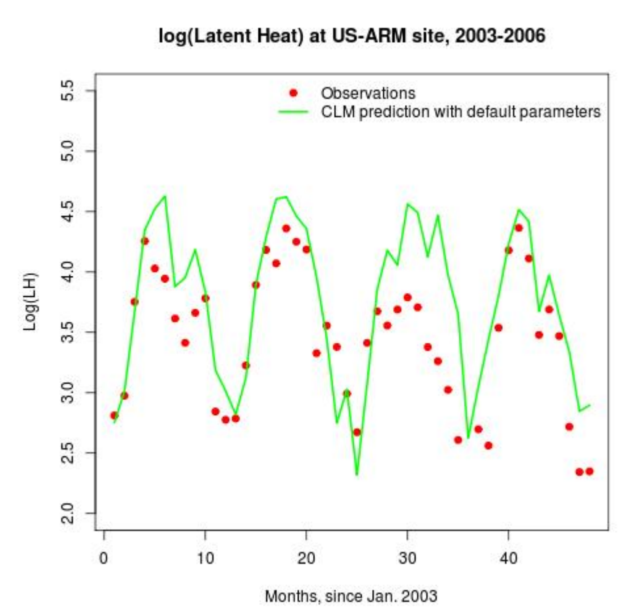
Perform a Bayesian calibration of three hydrological parameters in the Community Land Model (CLM)

- Use monthly-averaged observations of latent heat fluxes (LH) at the US-ARM site (Oklahoma) collected during 2003-2006 (48 months, total)
- Compute the uncertainty in the parameter estimates
- Model and compute the structural error in CLM; investigate sensitivity of the calibration to the choice of structural error model
- Investigate sensitivity of calibration to climatological averaging

TECHNICAL APPROACH

Inverse problem

- CLM comes with parameters set at certain default values; often not very predictive
- We seek to calibrate Θ = {F_{drai}, log(Q_{dm}), B}
  - F_{drai}: Decay factor for subsurface runoff with depth
  - Qdm: max subsurface drainage
  - B: Clapp and Hornberger exponent in the soil water retention curve



LH observation and CLM predictions with parameters set at default values

- Let y^{obs} be log(LH) observations and M(Θ) be the model
- $y^{obs} = M(\Theta) + \varepsilon$, $\varepsilon \sim \mathcal{N}(0, \Gamma)$ is a model-data mismatch modeled as a multivariate Gaussian because of time-correlated errors
- Our prior beliefs regarding parameters
  - $F_{drai} \sim \mathcal{U}(0.1, 5.0)$; default: 2.5
  - log(Q_{dm}) ~ $\mathcal{U}$(log(10^{-6}), log(10^{-2})); default : log(5.5 x 10^{-3})
  - B ~ $\mathcal{U}$(0.1, 15)

Bayesian formulation of the inverse problem

- Involves using Bayes' theorem to derive an expression for the probability density of Θ, conditioned on y^{obs}
- Using $\Pi(\Theta)$ to denote the prior distribution on Θ

$$P(\Theta \mid y^{obs}) \propto P(y^{obs} \mid \Theta)\Pi(\Theta)$$
$$= \left|\Gamma\right|^{-1/2} \exp\left[-\left(y^{obs} - M(\Theta)\right)^T \Gamma^{-1}\left(y^{obs} - M(\Theta)\right)\right]\Pi(\Theta)$$

- This is a 3-parameter estimation; higher dimension if we estimate Γ
- Will use an adaptive Markov chain Monte Carlo (MCMC) method [1] to compute estimates as a multidimensional posterior distribution.
- Will require O(10^5) evaluations of CLM
  - We need to make a surrogate of CLM if we desire a converged posterior distribution

CONSTRUCTING CLM SURROGATES

Surrogate models

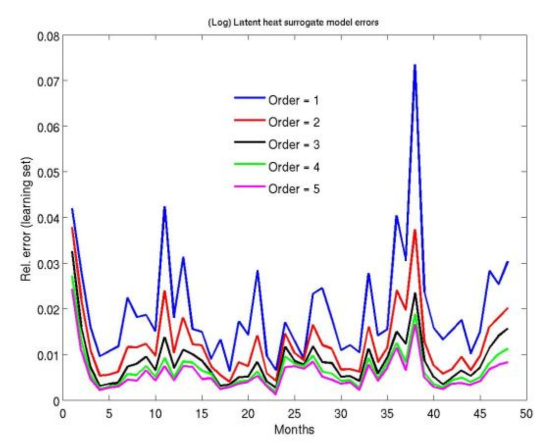
- Surrogate model – an inexpensive "curve fit" which approximates the input-output mapping by CLM of LH and Θ
- We propose a polynomial form

$$\log(LH) = \sum_{p=0}^{M} \sum_{q=0}^{M} \sum_{i=1}^{3} \sum_{j=1}^{3} w_{i,j}^{(p,q)} \theta_i^p \theta_j^q$$

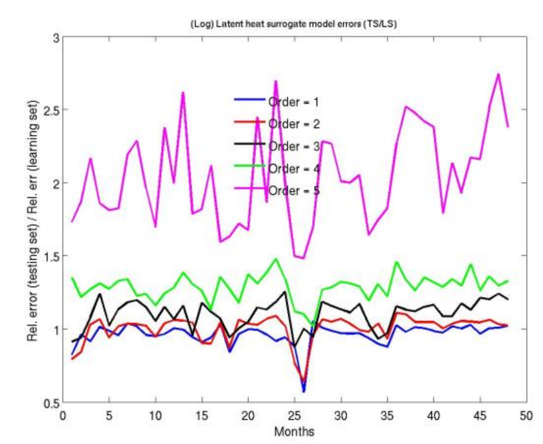
- $\Theta = \{\theta_1, \theta_2, \theta_3\}$ = {F_{drai}, log(Q_{dm}), B}; (p+q) < M
- Tested M = 1 … 5 to explore linear to 5^{th}-order models
- $w^{(p,q)}_{i,j}$ are estimated by linear regression to a training set of CLM runs

Selecting and configuring surrogates

- Sampled 256 points in the Θ-space (via space-filling quasi-Monte Carlo sampling) and generated 48-month time-series of log(LH) predictions
- Constructed polynomial models for each month
- Segregated 85% of the runs into a learning set (LS); estimated $w^{(p,q)}_{i,j}$ using linear regression
  - Used AIC to remove superfluous polynomial terms and prevent overfitting
- Used the remaining 15% of the runs as the testing set (TS); computed the RMS prediction error for the fitted polynomial model
- Repeated for 100 (LS/TS) pairs
- A good model should:
  - Have similar accuracy for LS and TS – else, we have overfitting
  - Have a small error (<10%) for LS



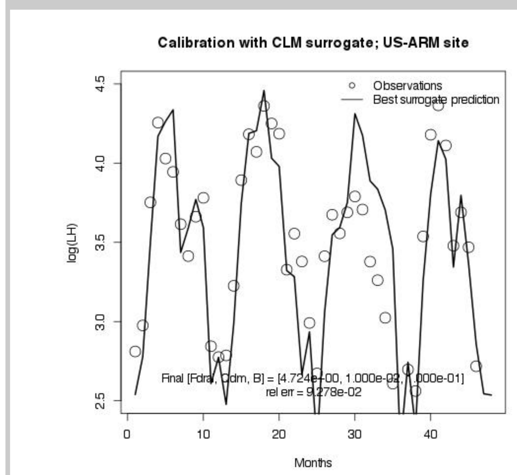
Learning set errors for surrogate models of order 1 to 5



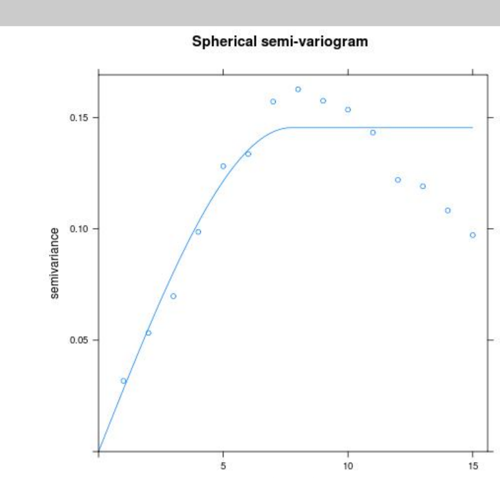
Ratio of LS / TS RMS errors for surrogate models of order 1 to 5

We chose quadratic models. Errors are < 4%

STRUCTURAL ERROR MODEL



Deterministic fit of CLM surrogates

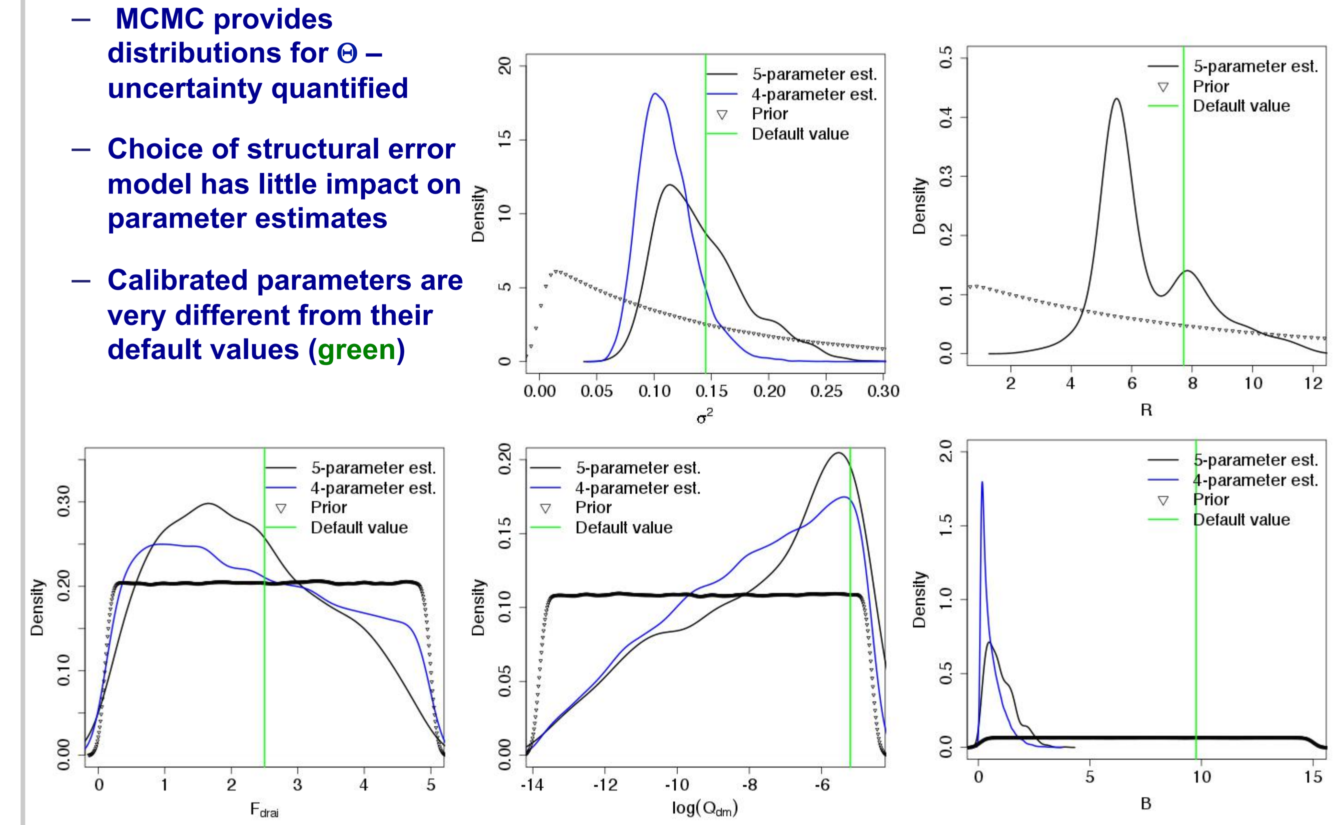


Spherical semi-variogram modeling

- A deterministic calibration of CLM surrogates revealed that the model-data mismatch may be correlated in time
- Correlation was modeled with a spherical semi-variogram; sill σ^2 = 0.145, range R = 7.72 months
  - Will henceforth use a spherical semi-variogram to model Γ

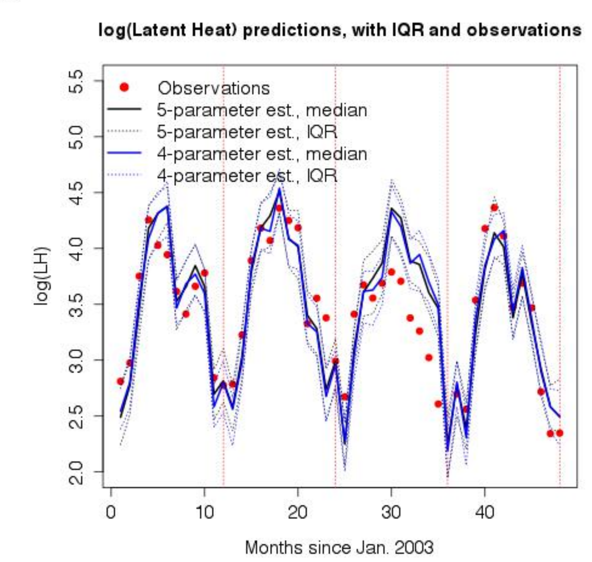
THE ESTIMATION PROBLEM

- 5-parameter estimation for {Θ, σ^2, R} [plotted in black]
  - Priors: σ^2 ~ Exp (mean = 0.145); R ~ Exp (mean = 7.72)
- A competing model: Assume data-model mismatch is NOT correlated in time (errors are i.i.d. Gaussians); estimate a 4-dimension problem for {Θ, σ^2} [plotted in blue]
  - Prior: σ^2 modeled with conjugate prior (inverse Gamma distribution)
- MCMC provides distributions for Θ – uncertainty quantified
- Choice of structural error model has little impact on parameter estimates
- Calibrated parameters are very different from their default values (green)



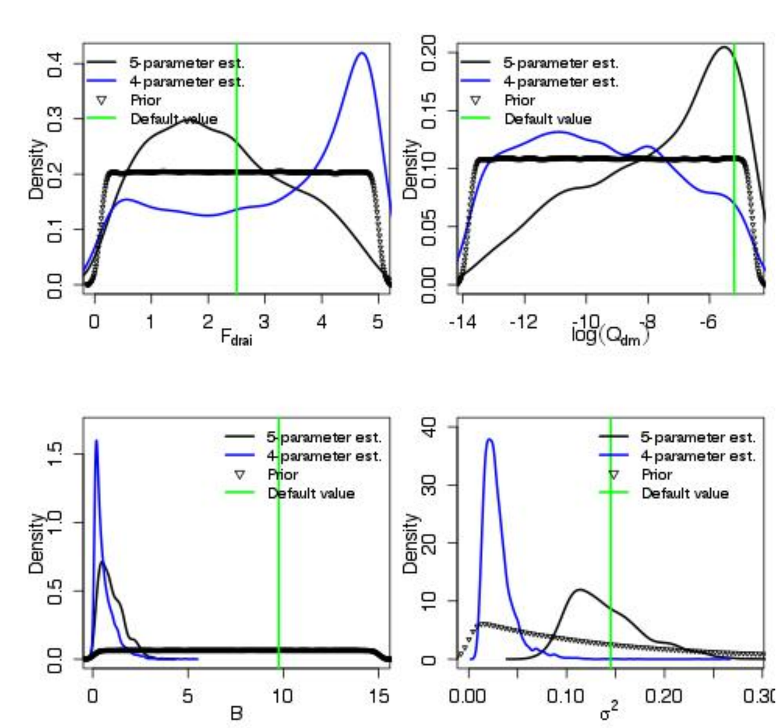
Predictive skill of calibrated model

- Both models (calibrated with and without time-correlated structural errors) are equally predictive
- And a big improvement over default values of the parameters
- The time-uncorrelated errors are preferable – much simpler



IMPACT OF CLIMATOLOGICAL AVERAGING

- Compute monthly average of LH for observations and CLM predictions
- Remake surrogates for 12 months; re-calibrate
- Figure (right) plots the PDFs for Θ
- Climatological averaging makes an enormous difference in F_{drai} and Q_{dm} calibrations
- Also B is still very different from default value
- Finally, the calibration error (σ^2) is far smaller than when calibrating to a 48-month time-series
  - We should expect this calibration to be far more predictive

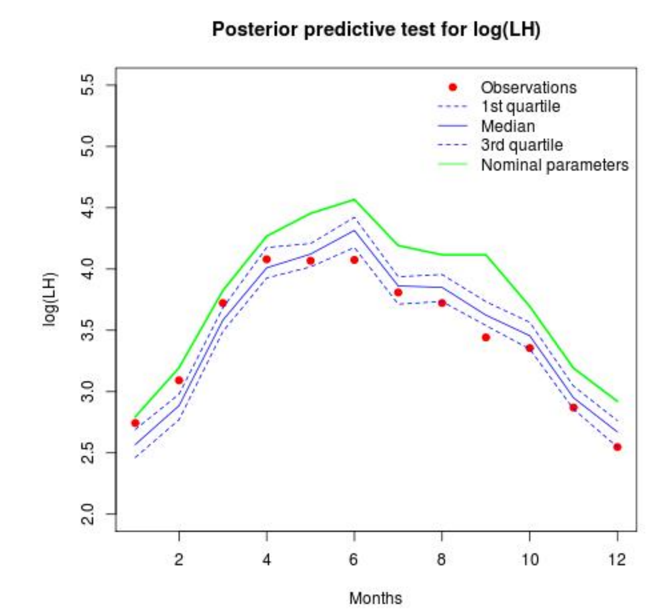


Comparison of PDFs of Q generated before (black) and after (blue) climatological averaging. The default values are in green

POSTERIOR PREDICTIVE TEST

Predictive skill of calibrated model after climatological averaging

- The calibration is far more predictive than before
- Reflected in the calibrated value of σ^2
- Not clear if this is due to a smaller σ^2 or better/sharper calibration of Θ
- But a huge improvement over the predictive skill of the uncalibrated model



CONCLUSIONS

- Surrogate models can allow efficient Bayesian calibration of CLM parameters
- The calibration is done with MCMC – it provides parameters as a joint probability density distribution
  - Automatically quantifies uncertainty in the estimates
  - Allows inference of structural error, magnitude and form
- For the US-ARM site, we find
  - 2 out of 3 hydrological parameters are very different from their default values
  - Choice of structural error model has very little impact
  - Climatological averaging has a huge impact on the calibration; it becomes more predictive as annual variations are averaged out
  - But climatological averaging still doesn't get the calibrated parameter values closer to the default ones

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References

1. H. Haario, M. Laine and A. Mira, "DRAM: Efficient adaptive MCMC", Statistical Computing, 16:339-354, 2006.

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