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Introduction

- Aim: Calibrate the Community Land Model (CLM) using timeseries measurements of latent heat and runoff
 - Bayesian calibration of 3 hydrological parameters w/ uncertainty
 - Estimate structural error (model-form error)
 - Compare with calibration done with each data type individually
- Site
 - US-MOz (latent heat) and MOPEX site # 7186000 (runoff)
- Why?
 - Structural error impairs a model's ability to reproduce all observables well
- Challenges
 - CLM is expensive 45 minutes/invocation per site;
 - No. of model invocation needed for Bayesian calibration = $O(10^4)$



What is CLM?

- A model for biogeochemical & hydrological processes
- Used in Earth system models; coupled to an atmosphere & ocean model
- Can be used in global (gridded) mode or locally for a site ("bucket" mode); can be driven by real meteorology
- Distributed by NCAR; has hard-coded parameters ("nominal values") which are meant to provided good global predictions
- When used in local mode, the parameters have to re-calibrated to be representative of local hydrological and biogenic processes
 - But it is not known whether calibrating to 1 data stream (e.g. latent heat) makes it predictive for all other observables
 - This is a type of structural error



What is structural error?

- The fundamental inability of a model to reproduce observations
 - Caused by missing physics in the model
- Previous work¹ has shown that calibrating to latent heat (LH) observations makes CLM predictive for LH
 - And it has a modest structural error that can be modeled as i.i.d.
 Gaussians
 - This does not show if the calibrated model can reproduce other observables like runoff
- This study
 - Calibrate using runoff; see what parameter estimates are like and how well we reproduce runoff
 - Then calibrate jointly on runoff and LH and see whether we still reproduce observations well
 - And how far the parameter estimates are from nominal values



¹Ray et al, Bayesian calibration of the Community Land Model using surrogates, SIAM J. Unc. Quant., accepted January 2015

The observations

- Data covers 2004-2007, 48 months
- Latent heat (LH) observations, Y^(obs)LH
 - Obtained from US-MOz a site in Missouri Ozark mountains
 - Averaged monthly, and then climatologically averaged to provide a 12-month time-series
- Runoff observations, Y^(obs)_{WPC}
 - Very noisy and not very useful as-is
 - We take a wavelet transform and use the amplitude-squared (wavelet power) at each time-scale as the observations
 - Called wavelet power curve (WPC)
 - We retain time-scales between 21 days and 4 years for calibration
- Sensitivity analysis showed that LH and WPC are most sensitive to 3 hydrological parameters – p = {F_{drai}, Q_{dm}, S_y}
 - These will be our calibration variables



Bayesian inference

- Model paramters p = {F_{drai}, log₁₀(Q_{dm}), S_y} estimated with the model errors
 - $Y^{(obs)}_{LH} = M_{LH}(p) + \varepsilon_{LH}, \varepsilon_{LH} \sim N(0, \sigma^2_{LH})$
 - $Y^{(obs)}_{WPC} = M_{WPC}(p) + \varepsilon_{wpc}, \ \varepsilon_{wpc} \sim N(0, \ \sigma^2_{wpc})$
 - σ^{2}_{ii} i ϵ {LH, WPC} is a crude measure of structural error in CLM
- Our prior beliefs (PDFs) for each parameter in {F_{drai}, log₁₀(Q_{dm}), S_y} are independent, uniform distributions with prescribed upper & lower bounds
- Posterior distribution P(p, σ^2_{LH} , σ^2_{WPC} | Y^(obs)_{LH}, Y^(obs)_{WPC})

$$P(F_{drai}, \log_{10}(Q_{dm}), S_{y} | Y_{LH}^{obs}, Y_{WPC}^{obs}) \propto \exp\left(-\frac{\left(Y_{LH}^{obs} - M_{LH}(p)\right)^{2}}{\sigma_{LH}^{2}} - \frac{\left(Y_{WPC}^{obs} - M_{WPC}(p)\right)^{2}}{\sigma_{WPC}^{2}}\right) \pi(p)$$

Solved using an adaptive Metropolis algo – DRAM



Surrogate models

- The inverse problem needs about 50K invocations of CLM
 - Can't be done today, so we make surrogates
- Surrogate details
 - We sample the $(F_{drai}, log_{10}(Q_{dm}), S_y)$ space with 282 points chosen via a quasi Monte Carlo space-filling method
 - CLM is run at these points; we save climatologically averaged predictions of LH and runoff
 - This is our training set
- Models are curve fits express Y = M(p)
 - You have to pick M and fit to data
 - You need some way to check against overfitting cross-validation, AIC etc.
 - Invariably latent heat or runoff needs to be transformed before being able to fit *M*



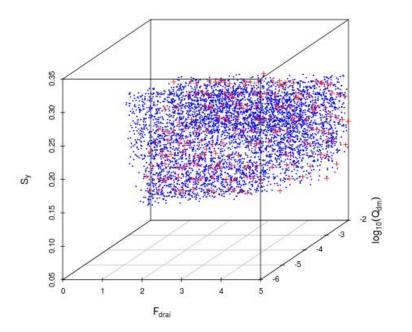
Latent heat surrogate models

- Transformations
 - 48 months of LH data is climatologically averaged, then log transformed
- Proposed a 5th order polynomial for $M_{LH}(p)$
 - Used AIC to simplify the model down to quadratic
 - Use randomized subsample validation tests to check for overfitting
 - Separate model for each month
 - The final fitted polynomial model has 10% 20% errors not good enough
- Regression kriging
 - Used quadratic as a mean/trend model and stationary Gaussian
 Process model around it (to combat 10%-20% discrepancy)
 - All models' errors dropped below 10%



Runoff surrogate models

- WPC surrogates
 - Surrogate could only be made for a subspace of (F_{drai}, log₁₀(Q_{dm}), S_y) space
 - Computed the MSE of each training run wrt observations & discarded the worst 25%
 - The retained parameters covered a region \mathcal{R} of the parameter space
 - Within \mathcal{R} , $M_{WPC}(p)$ could be modeled using quadratic polynomials
- We redefine our prior $-\pi(p) = 1, p \in \mathcal{R}, 0$ otherwise



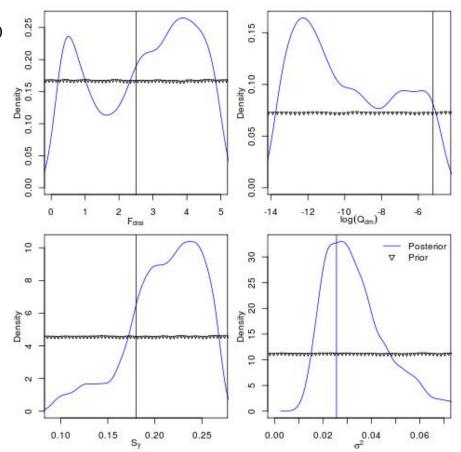
 ${\mathcal R}$ defined using a SVM classifier trained on selected & discarded runs in the training set



Calibration with LH data only

$$P(:|:) \propto \exp\left(-\frac{\left(Y_{LH}^{obs} - M_{LH}(p)\right)^{2}}{\sigma_{LH}^{2}} - \frac{\left(Y_{WPC}^{obs} - M_{WPC}(p)\right)^{2}}{\sigma_{WPC}^{2}}\right) \pi(p)$$

- The PDFs are not very well defined (bi-modal etc.)
- There is not much support for the nominal values of parameters





Reproducing observations

(HJ) go

2

- Pick 100 samples from the posterior density
- Run CLM for each
- Plot ensemble of predictions
- The variation in log(LH) predictions is tiny
 - Can't see the error bars around the circles
 - Explains why it was so difficult to find a sharp posterior distribution

4.5 4.0 3.5 3.0 Prediction 5.0 Observations

Nominal

Months

6

8

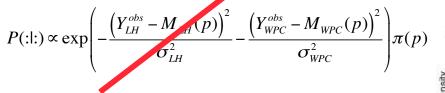
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12

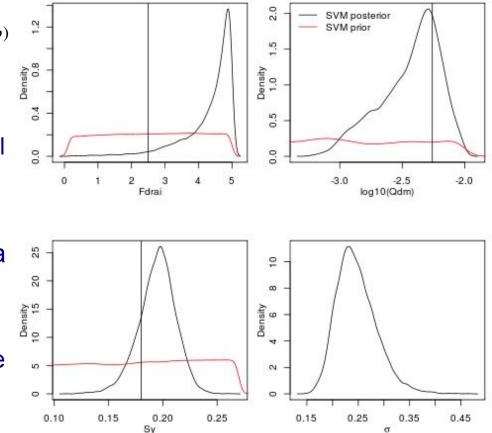
approxim

log(LH) pushed forward posterior

Calibration with WPC data only



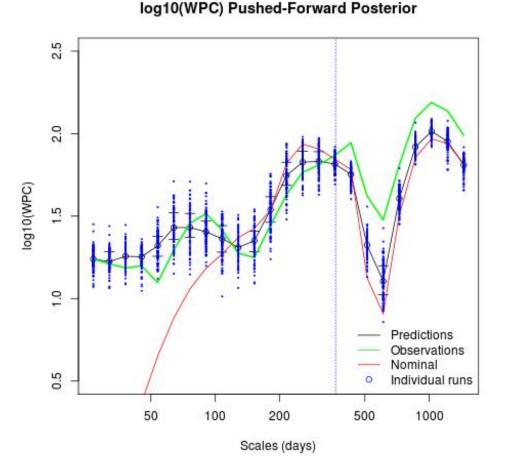
- The PDFs are simple
 - Not much support for nominal
 F_{drai}
- PDFs very different from the ones estimated using LH data only
 - First indication that it takes very different estimates of the parameters to match LH and WPC data





Reproducing observations

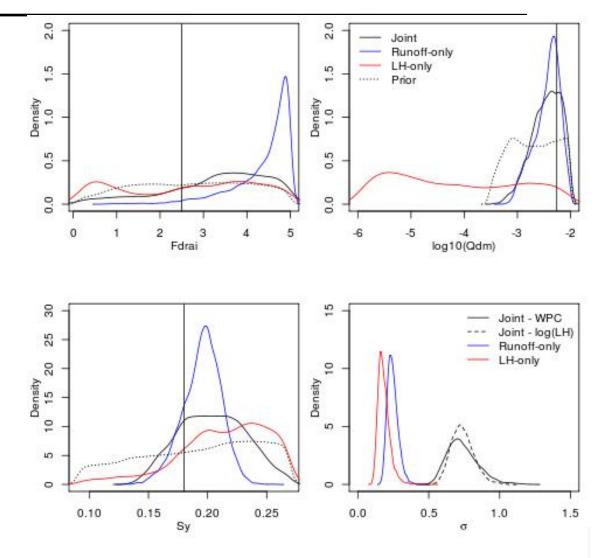
- Lots of scatter in predictions at small temporal scales
- But calibrated model's predictive skill better than nominal values of the parameters





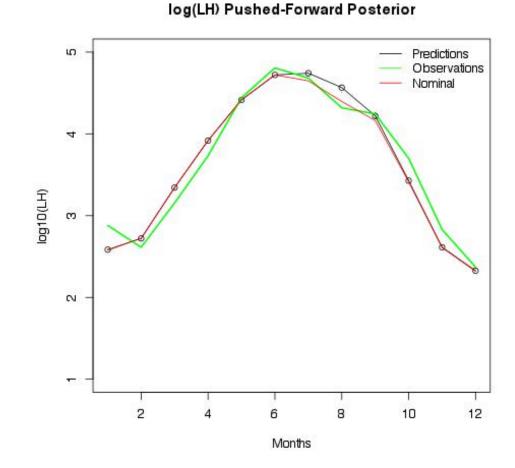
Joint calibration to LH and WPC data

- Huge change in PDFs
 - F_{drai} affects LH much, so joint and LH-only calibration are similar
 - Qdm affects WPC much, and so joint and WPC-only calibration similar
 - S_y well, your pick
- And the structural error is 6x larger
 - We simply can't be very predictive



Reproducing LH observation with CLM

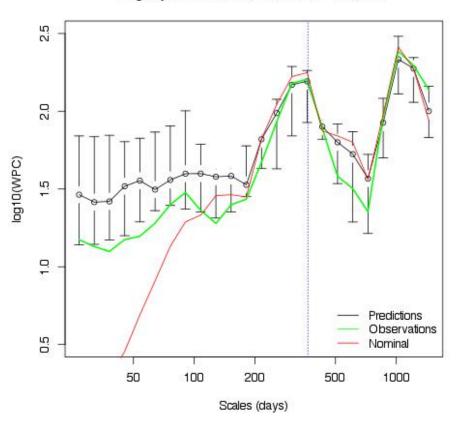
- Hardly any variability
 - LH predictions not at all sensitive to posterior
 - No wonder we could not get useful PDFs our of LH-only calibration





Reproducing WPC observation with CLM

- Good variability
 - Observations contained in inter-quartile "error bars"
- Big improvement in predictions at monthly timescales
 - Should be enough to resolve seasonal variations



log10(WPC) Pushed-Forward Posterior

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Conclusions

- CLM can be calibrated to reproduce a given datastream well
 - The model form error so obtained is too optimistic
 - And the parameters estimates are wrong
- Joint calibration with 2 types of data uncovers a second type of structural error
 - Its inability to reproduce multiple observations stream accurately
 - The parameter estimates obtained from 2 data streams have some resemblance to their nominal values
- Related talks
 - L. Swiler, MS 164, Room 251, Monday, 2:20pm 2:50pm [On the perils of parameter estimation using surrogates of CLM]
 - Z. Hou, CP 16, Room 254B, Wednesday, 9:25am 9:35am [On the applicability of parameter estimated from one site, to other similar sites; called "transferability"]

