Statistical Methods for Ice Sheet Models

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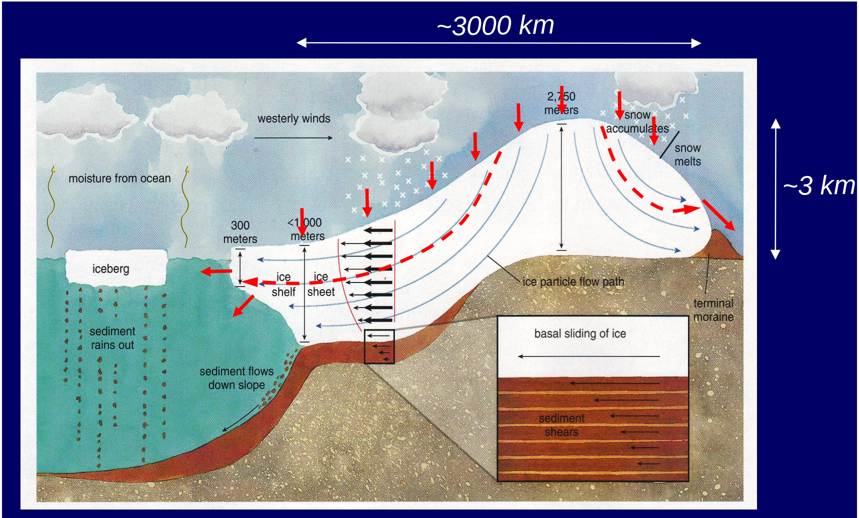
Talk Summary

- The West Antarctic Ice Sheet (WAIS) has the potential to be a significant contributor to future sea level change.
- How can we project the future behavior of WAIS? One approach: PSU-ICE model (Pollard and DeConto, 2009).
- Uncertain about key model input parameters.
- Our research: methods to use observations of the ice sheet to infer parameters.
- Challenges
  1. spatial binary/non-Gaussian data
  2. high-dimensional
  3. data-model discrepancies
- I will describe methods to address these issues.

Ice Sheet Physics

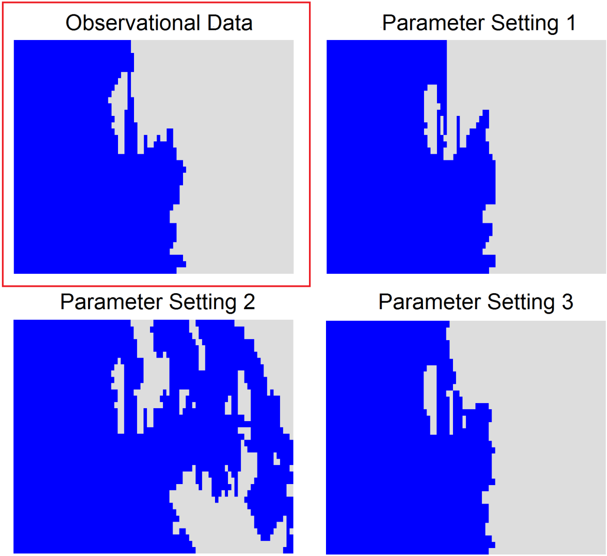


Siegert, 2002, Amer. Sci.

Ice Sheet Model Parameters

- The ice sheet's behavior is complex.
- Model equations predict ice flow, thickness, temperatures, and bedrock elevation, through thousands to millions of years.
- Examples of key model parameters:
  - Ocean melt coefficient: sensitivity of ice sheet to temperature change in the surrounding ocean
  - Strength of the "calving" process. Calving = where ice breaks off and transitions from attached to floating
  - "Slipperiness" of the ocean floor

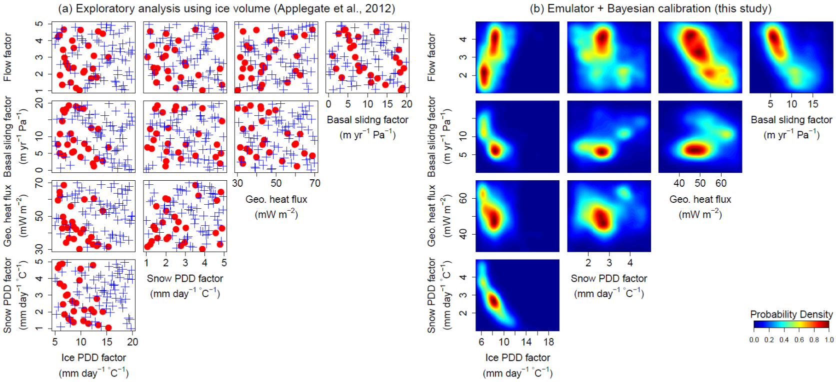
West Antarctic Ice Sheet Example



How Does Statistical Rigor Help Scientists?

1. We account for (epistemic) uncertainties in emulation
2. We provide *real* probability distributions, very important for impacts/risk quantification.
3. We use all available information (no aggregation): often reduces uncertainties.
4. We provide sharper/more useful results.

Example of Sharper Results



Left: previous ad-hoc methods. Right: statistical calibration

Two-stage Approach to Emulation-Calibration

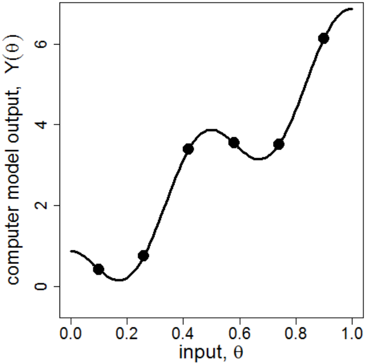
Outline of our approach

1. Emulation step: Find fast approximation for computer model using a Gaussian process (GP).
2. Calibration step: Infer climate parameter using emulator and observations, while accounting for data-model discrepancy

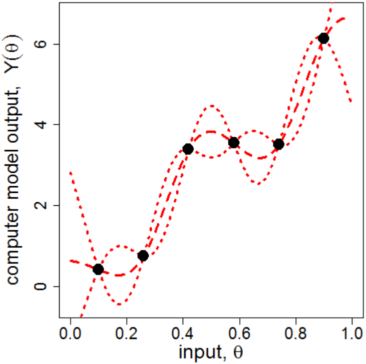
- Two stage: Liu, Bayarri and Berger (2009), Bhat, Haran, Olson, Keller (2012)
- Joint model approach: Sanso et al. (2008); Higdon et al. (2008).

Emulation Step

Toy example: model output is a scalar, and continuous.



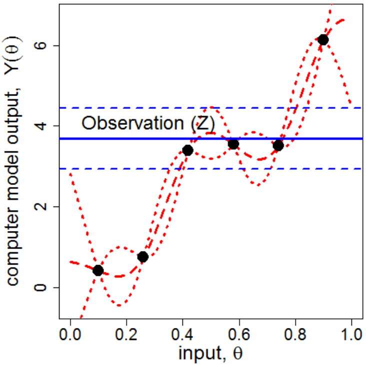
Computer model output (y-axis) vs. input (x-axis)



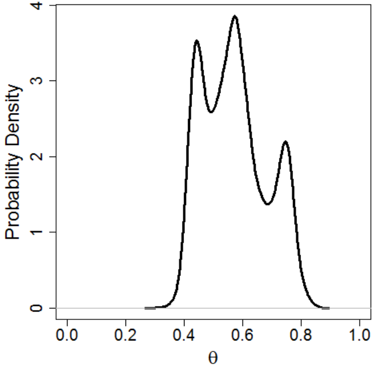
Emulation (approximation) of computer model using GP

Calibration Step

Toy example: model output, observations are scalars



Combining observation
and emulator



Posterior PDF of θ
given model output and observation

Summary of Statistical Problem

- **Goal**: Learn about θ based on two sources of information:
  - **Observations**: $\mathbf{Z} = (Z(\mathbf{s}_1), \ldots, Z(\mathbf{s}_n))^T$, where $\mathbf{s}_1, \ldots, \mathbf{s}_n$ locations (1D, 2D or 3D)
  - **Model output** $\mathbf{Y}(\theta_1), \ldots, \mathbf{Y}(\theta_p)$, where each $\mathbf{Y}(\theta_i) = (Y(\theta_i, \mathbf{s}_1), \ldots, Y(\theta_i, \mathbf{s}_n))^T$ is a vector of spatial data

Step 1: Computer Model Emulation Basics

- Fit Gaussian process model for computer model output **Y** to interpolate the values at the parameter settings $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_p$ *and* the spatial locations $\mathbf{s}_1, \ldots, \mathbf{s}_n$

$$\text{vec}\,(\mathbf{Y}) \sim N(\mathbf{X}\beta, \boldsymbol{\Sigma}(\xi_y)),$$

  vec($\cdot$) concatenates columns into one vector
- β and ξ_y estimated by maximum likelihood, $\hat{\beta}, \hat{\xi}_y$.
- Covariance interpolates across spatial surface *and* input space.

Result: Obtain a probability model (= predictive distribution) for model output at any input parameter θ, $\eta(\boldsymbol{\theta}, \mathbf{Y})$.

Step 2: Calibration Basics

- Discrepancy $\approx$ mismatch between computer model output and data when parameters are perfectly calibrated and there is no observational error.
- Probability model for observations $\mathbf{Z}$ is then

$$\mathbf{Z} = \eta(\boldsymbol{\theta}, \mathbf{Y}) + \boldsymbol{\delta},$$

where n-dimensional spatial field $\boldsymbol{\delta}$ is model-observation discrepancy with covariance parameter $\boldsymbol{\xi}_\delta$.

- Inference for $\boldsymbol{\theta}$ based on posterior distribution

$$\pi(\boldsymbol{\theta}, \boldsymbol{\xi}_\delta | \mathbf{Z}, \mathbf{Y}, \hat{\boldsymbol{\xi}}_y) \propto \underbrace{\mathcal{L}(\mathbf{Z} | \mathbf{Y}, \boldsymbol{\theta}, \boldsymbol{\xi}_\delta, \hat{\boldsymbol{\xi}}_y)}_{\text{likelihood given by above}} \times \underbrace{p(\boldsymbol{\theta}) \times p(\boldsymbol{\xi}_\delta)}_{\text{priors for } \boldsymbol{\theta} \text{ and } \boldsymbol{\xi}_\delta}$$

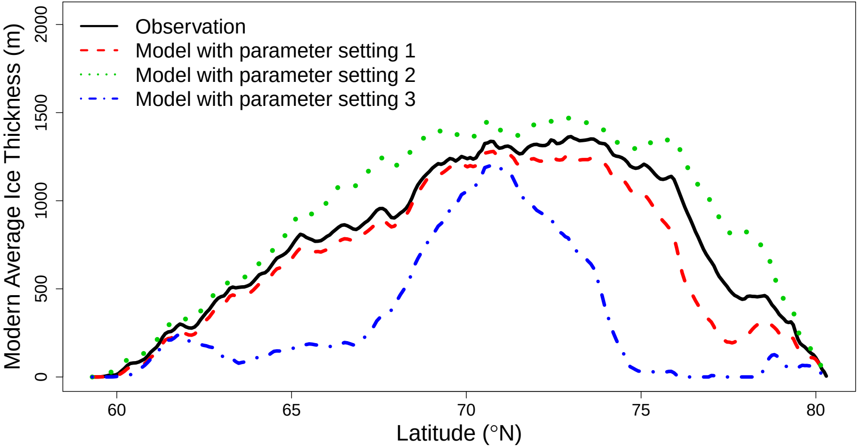
with emulator parameter $\hat{\boldsymbol{\xi}}_y$ fixed at value estimated in emulation step.

Why Data Aggregation is Popular

- The approach outlined works except for the computational issues posed by the size of the data.
- Can side-step computational problems by aggregatoin:
  - Computational problem solved.
  - Often more amenable to Gaussian process models.
  - Sometimes justified by the models: may only be appropriate (have “good skill”) at an aggregate level.

Example: Aggregated Greenland Ice Sheet Data

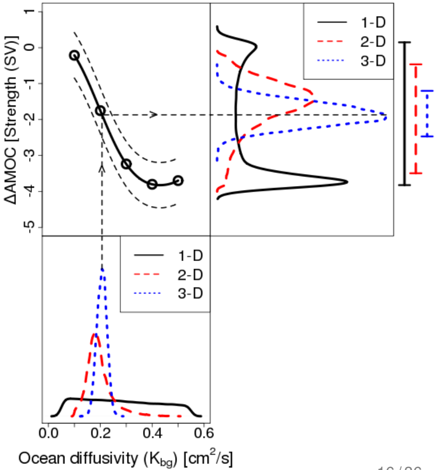
- To avoid binary spatial data: aggregate across longitude.



Avoid Aggregation to Reduce Uncertainties

(Chang, Haran, Olson, Keller, 2014)
In some cases, obtain sharper results if we can avoid aggregation.

- We compare 1D (depth profile) and 2D (zonal average) with 3D (unaggregated) data.
- Inference with 3D data leads to sharper inference for $\boldsymbol{\theta}$.
- Inference using 3D data is more robust to changes in prior specifications for discrepancy parameters.



Emulation-Calibration with Binary Spatial Output

- Now $Y(\boldsymbol{\theta}, \mathbf{s})$ is binary (0-1) model ouput, $Z(\mathbf{s})$ is data.
- Let $\mathbf{\Gamma}_{p \times n}$ be matrix of natural parameters for model output: $\gamma_{ij}^{Y} = \log\left(\frac{p_{ij}}{1-p_{ij}}\right)$ is logit for ith parameter setting at jth spatial location and $p_{ij} = P(Y(\boldsymbol{\theta}_i, \mathbf{s}_j) = 1)$.
- Given $\mathbf{\Gamma}$, $Y(\boldsymbol{\theta}_i, \mathbf{s}_j)$'s are conditionally independent Bernoulli.
- Approach (sketch):
  1. Assume it is possible to estimate $\mathbf{\Gamma}$ from the $n \times p$ matrix of computer model output.
  2. Emulate computer model by *interpolating natural parameters* using a Gaussian process across input parameter space and spatial locations.
  3. Calibration by using fitted Gaussian process $\eta(\boldsymbol{\theta}, \mathbf{Y})$ + discrepancy δ to obtain a likelihood function for the *natural parameter vector for observations*.

Challenges

- Step 1 (obtaining $\boldsymbol{\Gamma}$) is ill-posed: *np* parameters for *np* data points.
- Step 2 (emulation) is computationally infeasible: Cholesky factorization has computational cost of $\frac{1}{3} \times p^3 \times n^3 = \frac{1}{3} \times 499^3 \times 3,182^3 = 1.33 \times 10^{18}$ flops
- Step 3 (calibration): involves having to perform a high-dimensional integration + expensive matrix operations.

We propose dimension-reduction to address both ill-posedness and computational issues.

Principal Components for Emulation: Basic Idea

- Consider model outputs at $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_p$ as if they were replicates of a multivariate process, thereby obtaining their PCs

$$\begin{pmatrix} Y(\mathbf{s}_1, \boldsymbol{\theta}_1) & \ldots & Y(\mathbf{s}_n, \boldsymbol{\theta}_1) \\ \vdots & \ddots & \vdots \\ Y(\mathbf{s}_1, \boldsymbol{\theta}_p) & \ldots & Y(\mathbf{s}_n, \boldsymbol{\theta}_p) \end{pmatrix}_{p \times n} \Rightarrow \begin{pmatrix} Y_1^R(\boldsymbol{\theta}_1) & \ldots & Y_{J_y}^R(\boldsymbol{\theta}_1) \\ \vdots & \ddots & \vdots \\ Y_1^R(\boldsymbol{\theta}_p) & \ldots & Y_{J_y}^R(\boldsymbol{\theta}_p) \end{pmatrix}_{p \times J_y}$$

- PCs pick up characteristics of model output that vary most across input parameters $\theta_1, \ldots, \theta_p$.
  Surprisingly flexible approach, including non-separable covariance.

Emulation Using PCs

Simple case: everything is well modeled by Gaussian processes.

- Fit 1-dimensional GP for each series $Y_j^R(\boldsymbol{\theta}_1), \ldots, Y_j^R(\boldsymbol{\theta}_p)$
- $\boldsymbol{\eta}(\boldsymbol{\theta}, \mathbf{Y}^R)$: J_y-dimensional emulation process for PCs, $\mathbf{Y}^R$ is collection of PCs
- Computation reduces from $\mathcal{O}(n^3p^3)$ to $\mathcal{O}(J_yp^3)$ (1.2×10^{21} to 1.0×10^8 flops).
- Emulation for original output: compute $\mathbf{K}_y\boldsymbol{\eta}(\boldsymbol{\theta}, \mathbf{Y}^R)$ where $\mathbf{K}_y$ is matrix of scaled eigenvectors
- Flexible emulator

Dimension Reduction for Discrepancy Process

- Kernel convolution: Specifying n-dimensional discrepancy process δ using J_d-dimensional knot process $\boldsymbol{\nu}$ ($J_d < n$) and kernel functions
- Kernel basis matrix $\mathbf{K}_d$ links grid locations $\mathbf{s}_1, \ldots, \mathbf{s}_n$ to knot locations $\mathbf{a}_1, \ldots, \mathbf{a}_{J_d}$;

$$\{\mathbf{K}_d\}_{ij} = \exp\left(-\frac{g(\mathbf{s}_i, \mathbf{a}_j)}{\phi_d}\right)$$

  with $\phi_d > 0$. Fix ϕ_d at large value determined by expert judgment
- Results in better identifiability: Overly flexible discrepancy process may be confounded with emulator

Efficient Emulation: Outline

More complicated case: binary spatial data.

- Think in terms of generalized linear mixed models.
- Rewrite $\boldsymbol{\Gamma}$ in terms of logistic principal components (Lee et al., 2010).
- Use maximum likelihood to perform logistic principal components. Non-trivial, requires majorization-minimization (MM) algorithm (Lange et al. 2000; Hunter and Lange, 2004).
- Emulate each column of (reduced-dimensional) principal component matrix with an independent Gaussian process. Very fast and easy to do.
- We can obtain an emulator for $\boldsymbol{\Gamma}$ by emulating these principal components.

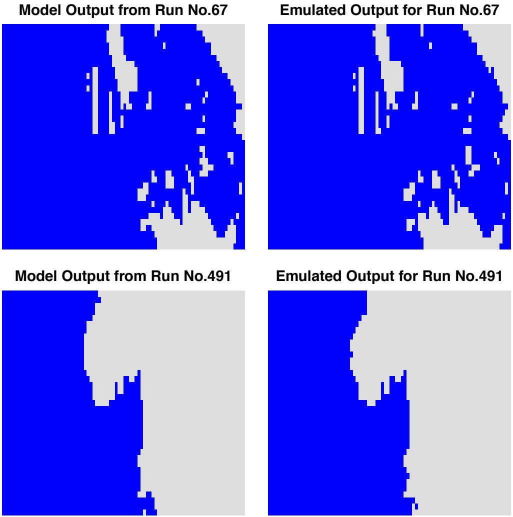
Dimension-reduction

- Consider $\mathbf{\Gamma}$ the $p \times n$ matrix of natural parameters for model output. Using logistic principal components (Lee et al., 2010), rewrite as:

$$\mathbf{\Gamma} = \mathbf{1}_p \otimes \boldsymbol{\mu}^T + \mathbf{W}\mathbf{K}_y^T, \tag{1}$$

  where $\mathbf{K}_y$ is an $n \times J_y$ orthogonal basis matrix, $\mathbf{W}$ is the $p \times J_y$ principal component matrix with (i, j)th element $w_j(\boldsymbol{\theta}_i)$, and $\boldsymbol{\mu}$ is the $n \times 1$ mean vector.
- Non-trivial and computationally challenging optimization to obtain matrices $\mathbf{W}$, $\mathbf{K}_y$ by maximizing log-likelihood. Use majorization-minimization (MM) algorithm (Lange et al. 2000; Hunter and Lange, 2004).
- Emulate each column of $\mathbf{W}$ using a separate Gaussian process.
- (Analogous to Gaussian emulation) By emulating these principal components we can emulate the original process.

Emulation Examples



Efficient Calibration Outline

- Model for n-dimensional vector of natural parameters $\boldsymbol{\lambda}$ for observational data using emulator $\mathbf{K}_y\boldsymbol{\eta}(\boldsymbol{\theta}, \mathbf{W})$:

$$\boldsymbol{\lambda} = \boldsymbol{\mu} + \mathbf{K}_y\boldsymbol{\eta}(\boldsymbol{\theta}^*, \mathbf{W}) + \boldsymbol{\delta},$$

  $\boldsymbol{\delta}$ is discrepancy term that represents structural error between the model output and observational data.
- To get around the challenges in integrating out $\boldsymbol{\delta}$, use a basis representation.
- Discrepancy basis obtained from common discrepancy pattern across parameter settings.

Efficient Calibration: Details

- Calibration model for n-dimensional vector of natural parameters $\boldsymbol{\lambda}$ for observational data using the emulator $\mathbf{K}_y\boldsymbol{\eta}(\boldsymbol{\theta}, \mathbf{W})$:

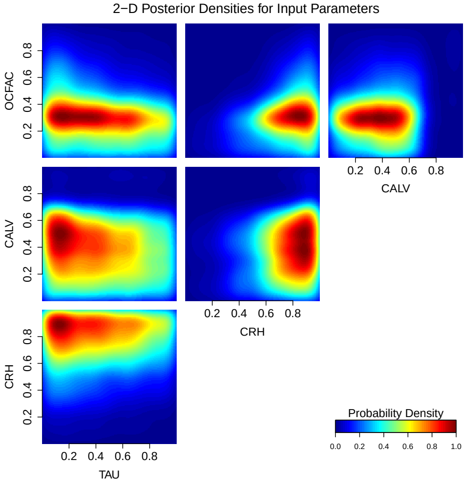
$$\boldsymbol{\lambda} = \boldsymbol{\mu} + \mathbf{K}_y\boldsymbol{\eta}(\boldsymbol{\theta}^*, \mathbf{W}) + \boldsymbol{\delta},$$

  where $\boldsymbol{\theta}^*$ is the "best fit" value for the observational data, $\boldsymbol{\delta}$ is discrepancy term that represents structural error between the model output and observational data.
- To get around the challenges in integrating out $\boldsymbol{\delta}$ described above we use a basis representation for the discrepancy term such that

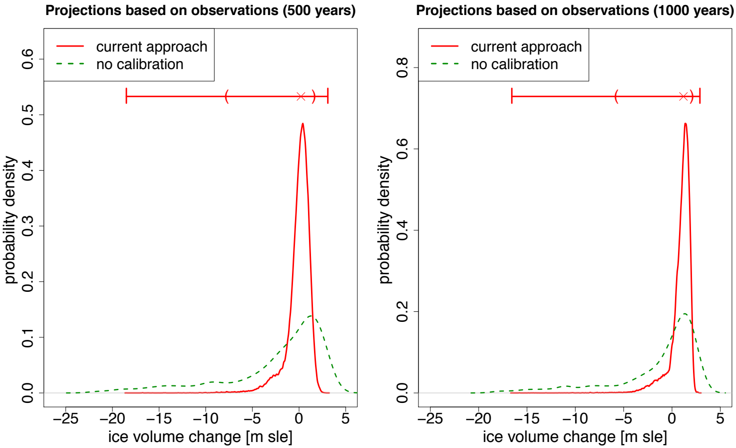
$$\boldsymbol{\delta} = \mathbf{K}_d\mathbf{v},$$

  with the $n \times J_d$ basis matrix $\mathbf{K}_d$ and the J_d-dimensional random coefficient vector $\mathbf{v} \sim N(\mathbf{0}, \sigma_d^2\mathbf{I}_{J_d})$.
- Discrepancy basis obtained from common discrepancy pattern across parameter settings, proportion mismatch at each location.

Calibration Results



Example Projections



Concluding Remarks

- I have described a computationally expedient approach for computer model emulation and calibration for high-dimensional binary spatial output.
- This tool is valuable for ice sheet model projections.
- Promising results when we incorporate paleo data.
- Caveats: we are using simple projection scenarios, we are ignoring floating ice information...
- Method tested extensively using simulated data examples, multiple data sets.
- Potentially useful for other (non-climate) complex computer model applications.

Acknowledgments

Collaborators:

- Won Chang, University of Chicago
- David Pollard, Earth and Environmental Systems Institute (EESI), Penn State U.
- Patrick Applegate, EESI, Penn State U.
- Klaus Keller, Geosciences, Penn State U.
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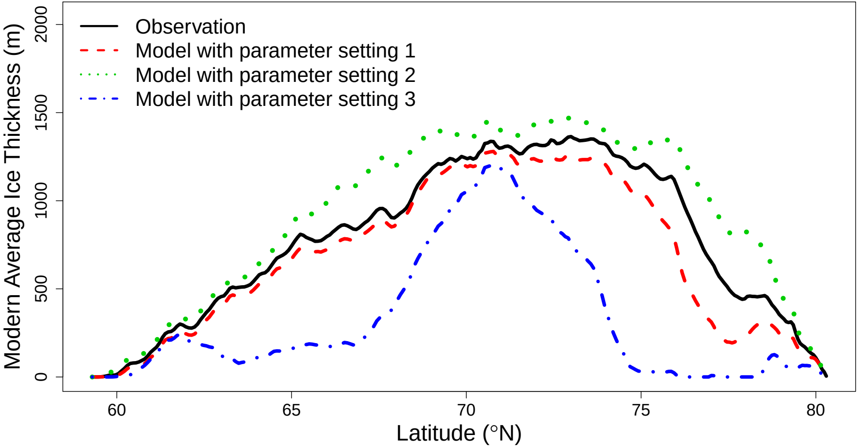
Relevant Manuscripts

- Chang, W., Haran, M, Applegate, P., Pollard, D. (2016): Calibrating an Ice sheet model using high-dimensional non-Gaussian spatial data, *Journal of the American Statistical Association*
- Chang, W., Haran, M, Applegate, P., Pollard, D. (2016): Improving Ice Sheet Model Calibration Using Paleoclimate and Modern Data, *on arxiv.org*.
- Chang, W., M. Haran, R. Olson, and K. Keller (2015): Fast dimension-reduced climate model calibration, *Annals of Applied Statistics*
- Chang, W., Applegate, P., Haran, M. and Keller, K. (2014) Probabilistic calibration of a Greenland Ice Sheet model using spatially-resolved synthetic observations: toward projections of ice mass loss with uncertainties, *Geoscientific Model Development*

Aggregated Ice Sheet Data: Example

- To avoid binary spatial data: aggregate across longitude.



Appendix Step 1: Emulation (Approximating Computer Model)

- Find MLE for covariance parameter $\boldsymbol{\xi}$, denoted by $\hat{\boldsymbol{\xi}}$
- Get $\boldsymbol{\eta}(\boldsymbol{\theta}_{NEW}, \mathbf{Y})$ for prediction at any $\boldsymbol{\theta}_{NEW} \in \Theta$:
  - GP gives

$$\begin{pmatrix} \mathbf{Y} \\ \mathbf{Y}(\boldsymbol{\theta}_{NEW}) \end{pmatrix} \sim N\left(\begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}_{n(p+1)\times 1}, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}_{n(p+1)\times n(p+1)} \right)$$

  - Emulator:

$$\boldsymbol{\eta}\left(\boldsymbol{\theta}_{NEW}, \mathbf{Y}\right) = \mathbf{Y}(\boldsymbol{\theta}_{NEW})|\mathbf{Y} \sim N\left(\Sigma_{21}\Sigma_{11}^{-1}\mathbf{Y}, \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}\right)$$

Appendix: Computational Challenges for Gaussian Emulation-Calibration

- Emulation requires dealing with $np \times np$ covariance matrix of $\mathbf{Y}$. E.g. if $n = 61,051$ $p = 250$
  - Cholesky decomposition costs $\frac{1}{3}n^3p^3 = 1.185 \times 10^{21}$ flops.
  - Covariance matrix is of size $8 \times \frac{250^2 \times 61051^2}{1024^3} = 1,735,624$
- Calibration faces similar challenges for dealing with $n \times n$ covariance matrix.

Our fast reduced-dimension approach: Fast computation using PC and Kernel Convolution

Appendix: What is the Effect of Data Aggregation?

- Common practice: Calibration using aggregated data (e.g. zonal average)
  - Avoiding computational issues
  - Limited skill of climate model in reproducing spatial patterns
- Using unaggregated data may result in
  - perhaps less uncertainty due to using more data?
  - perhaps more uncertainty due to poor model skill?
- Largely unanswered due to inability to handle unaggregated data

Appendix: Cross-Validation for Emulator

- Example of leave-10%-out cross validation result: