Inference with Implicit Likelihoods and High-dimensional Data

Murali Haran

Department of Statistics
Pennsylvania State University

joint with:
Won Chang (Statistics, Penn State)
Sham Bhat (Los Alamos National Labs)
Roman Olson (Geosciences, Penn State)
Klaus Keller (Geosciences, Penn State)

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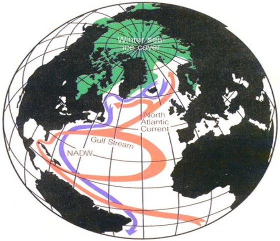
What This Talk is About

- Models for complex physical systems can be used to inform science and policy
  - Climate models: projections about future climate
  - Infectious disease models: design intervention strategies
- These models are based on the dynamics underlying the systems. Complicated and involve unknown parameters
- I will discuss “calibration” methods: how to use high-dimensional multivariate (spatial/space-time) observations of the system to infer unknown parameters

The Atlantic Meridional Overturning Circulation (MOC)



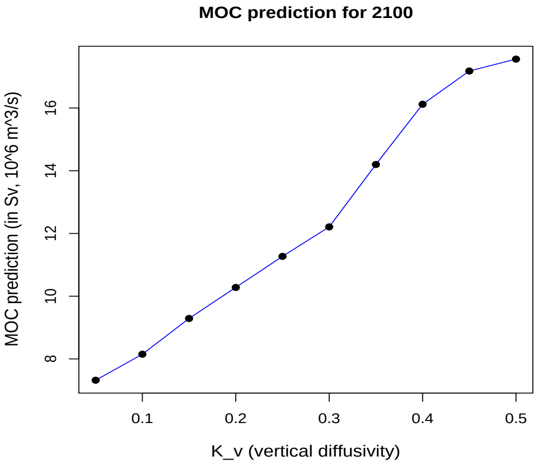
Rahmstorf (1997)

Global conveyor belt: carries warm upper waters into far-northern latitudes and returns cold deep waters southward across the equator

The MOC and Climate Change

- Its heat transport makes a substantial contribution to the moderate climate of Europe (cf. Bryden et al., 2005)
- Any slowdown in the overturning circulation would have profound implications for climate change
- Climate scientists use climate models to make projections about the MOC

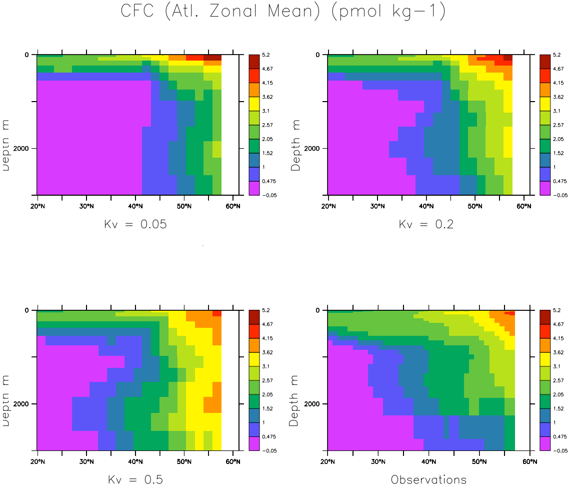
MOC Predictions and Model Parameter K_{bg}



Learning about $\mathbf{K_{bg}}$

- $\mathbf{K_{bg}}$ is a model parameter that quantifies the intensity of vertical mixing in the ocean. Cannot be measured directly
- Two sources of indirect information:
  - **Observations** of ocean "tracers" that provide information about $\mathbf{K_{bg}}$. Examples: $\Delta^{14}C$ and trichlorofluoromethane (CFC11) collected in the 1990s
  - **Climate model output** at different values of $\mathbf{K_{bg}}$ from University of Victoria (**UVic**) Earth System Climate Model (Weaver et. al., 2001)
- Each tracer has
  - 2D spatial observations: 3706 locations
  - 2D model output: 5926 locations *at each parameter setting*
- (Later) 3D spatial observations: 61,000 locations

CFC-11 Example: 2-D



Bottom right corner: observations

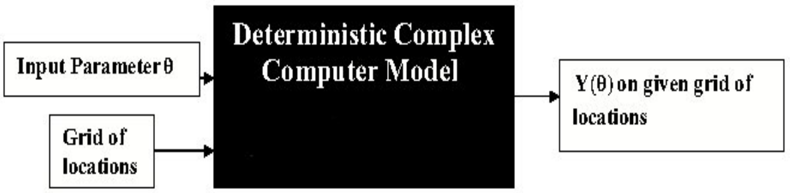
Other plots: climate model output at 3 settings of K_v

Challenges

This is a computer model calibration problem

1. The climate model is computationally intensive: can only be run at a few different settings
2. Output/observations are in the form of multivariate spatial data. (Toy e.g. was scalar!) Poses modeling, computational challenges
3. Combining information from tracers CFC-11, $\Delta^{14}C$: need a computationally tractable model for flexible relationships *between* the spatial fields.

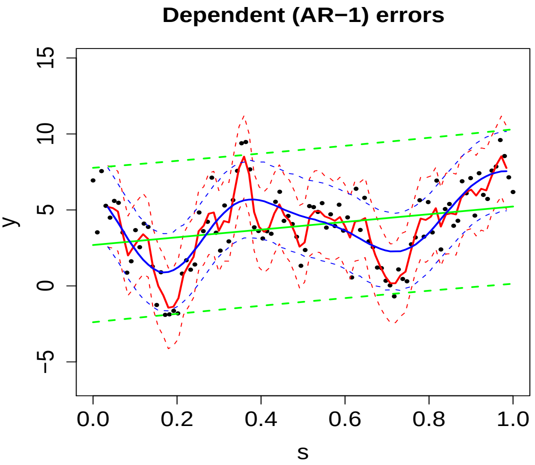
Computer Model Emulation



- Replace complicated computer model with a stochastic approximation: Gaussian process (Sacks et al., 1989)
- Gaussian process (GP) is an infinite-dimensional stochastic processes. Joint distribution of the process at any finite set of locations is multivariate normal
- For computer models “location” = parameter (θ) setting

Currin et al. (1991); Bayarri, Berger et al. (2007); Sanso et al. (2008)

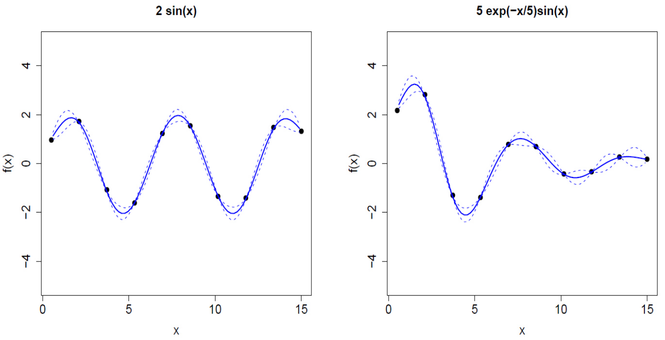
GP Model for Dependence: Toy 1-D Example



Black: 1-D AR-1 process simulation. Green: independent error.

Red: GP with exponential, Blue: GP with gaussian covariance.

GP Model for Emulation: Toy 1-D Example



Same simple model for both, $f(x) = \alpha + w(x)$ where $\{w(x),\ x \in (0, 15)\}$ is a Gaussian process

Notation

- $Z_1(\mathbf{s}), Z_2(\mathbf{s})$: tracer 1 and 2 at location $\mathbf{s}$=(latitude, depth). Let $\mathbf{Z}_1, \mathbf{Z}_2$ be the two spatial fields
- $Y_1(\mathbf{s}, \theta)$, $Y_2(\mathbf{s}, \theta)$: model output at $\mathbf{s}$, θ
  Let $\mathbf{Y}_1, \mathbf{Y}_2$ be the model output for the two tracers, spatial fields across multiple parameter settings

Goal: Inference for climate parameter θ using $\mathbf{Z}_1, \mathbf{Z}_2, \mathbf{Y}_1, \mathbf{Y}_2$.
We will exploit the fact that GPs can be used to model complicated functions and spatial data simultaneously

Two-Stage Computer Model Calibration

Our approach

1. **Emulation**: Model relationship between $\mathbf{Z} = (\mathbf{Z}_1, \mathbf{Z}_2)$ and $\boldsymbol{\theta}$ via emulation of model output.
   i An approximation to the computer model using $\mathbf{Y} = (\mathbf{Y}_1, \mathbf{Y}_2)$: $f(\mathbf{Y} \mid \boldsymbol{\theta})$
   ii Take above approximation + systematic model-data discrepancy + measurement error. This gives a model for the observations $\mathbf{Z}$: $f(\mathbf{Z} \mid \boldsymbol{\theta})$
2. **Calibration**: obtain posterior distribution of $\boldsymbol{\theta}$,

$$\pi(\boldsymbol{\theta} \mid \mathbf{Z}) \propto f(\mathbf{Z} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})$$

Step 1: Emulation with Multiple Spatial Fields

- Model $(\mathbf{Y}_1, \mathbf{Y}_2)$ as a hierarchical model: $\mathbf{Y}_1|\mathbf{Y}_2$ and $\mathbf{Y}_2$ as Gaussian processes (following Royle and Berliner, 1999)

$$\mathbf{Y}_1 \mid \mathbf{Y}_2, \boldsymbol{\beta}_1, \boldsymbol{\xi}_1, \gamma \sim N(\mu_{\boldsymbol{\beta}_1}(\boldsymbol{\theta}) + \mathbf{B}(\gamma)\mathbf{Y}_2, \Sigma_{1.2}(\boldsymbol{\xi}_1))$$

$$\mathbf{Y}_2 \mid \boldsymbol{\beta}_2, \boldsymbol{\xi}_2 \sim N(\mu_{\boldsymbol{\beta}_2}(\boldsymbol{\theta}), \Sigma_2(\boldsymbol{\xi}_2))$$

- $\mathbf{B}(\gamma)$ relates $\mathbf{Y}_1$ and $\mathbf{Y}_2$, with parameters γ
- *Covariance is a function of spatial distance and distance in parameter space*
- $\boldsymbol{\beta}$s, $\boldsymbol{\xi}$s are regression, covariance parameters

Flexible relationship between $\mathbf{Y}_1$ and $\mathbf{Y}_2$

Step 2: Calibration with Multiple Spatial Fields

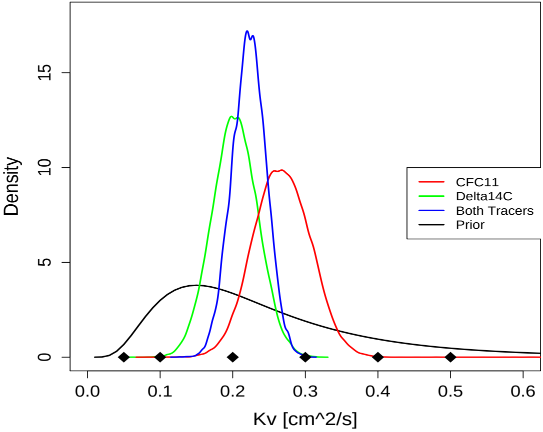
- Fit GP via maximum likelihood, then obtain predictive distribution at locations of observations
- Model observations by adding measurement error and a model discrepancy term to the GP emulator:

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

  where $\boldsymbol{\delta}(\mathbf{Y}) = (\boldsymbol{\delta}_1 \ \boldsymbol{\delta}_2)^T$ is the model discrepancy,
  $\boldsymbol{\epsilon} = (\boldsymbol{\epsilon}_1 \ \boldsymbol{\epsilon}_2)^T$ is the observation error
  Discrepancy can make crucial adjustments to $\boldsymbol{\theta}$ inference (Bayarri et al. 2007; Bhat et al., 2010)
- Markov chain Monte Carlo (MCMC) to obtain $\pi(\boldsymbol{\theta} \mid \mathbf{Z}, \mathbf{Y})$

Details: kernel mixing + patterned covariances for fast matrix operations; discrepancy function; MCMC algorithm

Results for K_v Inference



posteriors: only CFC-11, only $\Delta^{14}C$, both CFC-11 & $\Delta^{14}C$.

Result: **K_{bg}** pdf suggests weakening of MOC in the future.

Alternate Sources of Information

Can also learn about $\mathbf{K_{bg}}$ via sea temperatures

- Scientific interest: how does aggregation affect inference? At what spatial scale should we be looking at information?
- Statistical question: compare calibration based on 1-D, 2-D versus 3-D information
- Methodological issue: existing approaches (ours, Higdon et al. (2008); Sanso et al. (2008); Bayarri et al. (2008) etc.) do not apply to this 3D spatial data with 61,051 data points $\times$ 250 parameter settings

Fast Approach for High-dimensional Calibration

- Construct low-dimensional representation of model output $\mathbf{Y}$ and observations $\mathbf{Z}$
  - Find eigenvectors $\mathbf{K}_Y$ and corresponding principal components of model output. Low-dimensional representation of model output: $\mathbf{Y}_R$
  - Project $\mathbf{Z}$ on space spanned by $\mathbf{K} = [\mathbf{K}_y\ \mathbf{K}_d]$ where $\mathbf{K}_d$ is kernel basis for discrepancy. Low-dimensional representation: $\mathbf{Z}_R$, still accounting for discrepancy
- Emulation and calibration as before, but with $\mathbf{Y}_R, \mathbf{Z}_R$
- Very fast compared to other methods, scales well
- Details: determining discrepancy basis, # of PCs, ...

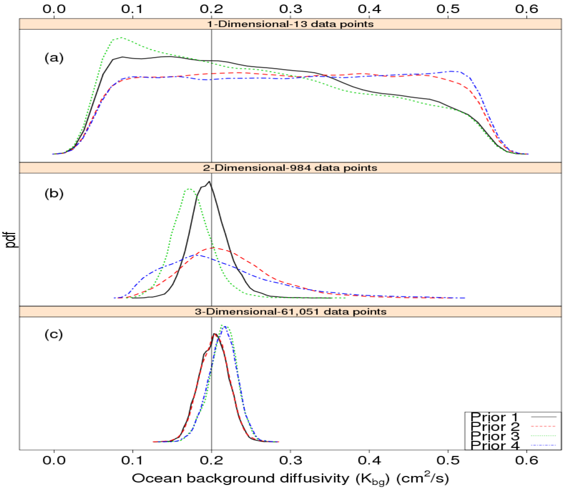
Simulated Example

Studied several simulated examples. Most challenging:

- Synthetic truth: 3-D model output at K_{bg} = 0.2
- Pseudo-residual= averaged residuals between data and model at a few settings. This is more sensible, realistic, challenging than simulating from various error models (cf. Jim Hodges' recent work)
- Pseudo observational data in 3D= synthetic truth + pseudo-residual
- Aggregate 3-D pseudo observations to get 2-D and 1-D

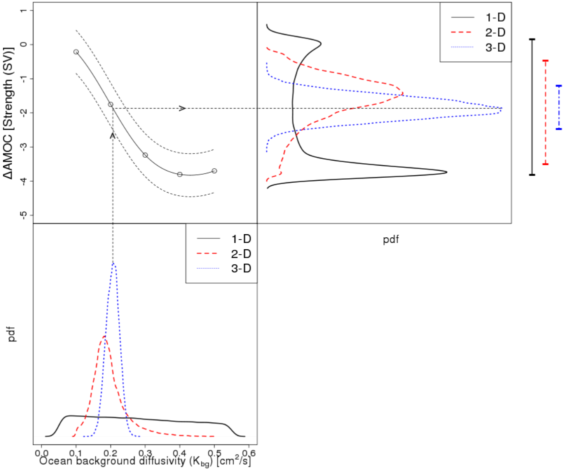
Compare inference based on 1D, 2D and 3D

Effect of Aggregation on Inference

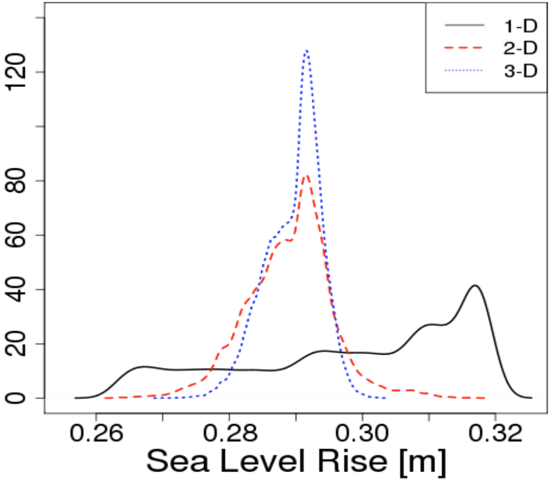


Simulated example: Unaggregated 3-D data (1) has sharpest posterior pdf and (2) most robust to changes in prior

MOC Projections for 2100 Using Inferred K_{bg}



Sea Level Rise Projections for 2100 Using Inferred K_{bg}



Summary

- Calibration with multivariate spatial data
  - Flexible hierarchical model
  - Kernel mixing/patterned covariances and matrix identities (e.g. Sherman-Woodbury-Morrison) for fast computing
  - Reliability of approach was studied extensively
- Calibration with high-dimensional spatial data
  - Fast dimension-reduced approach
  - Works well in practice
  - Allows first time calibration with 3D spatial data
  - Unaggregated data is better for inference
- Regardless of tracers, aggregation, model or methods: MOC projected to weaken in the future
- (Not discussed here) General calibration framework applied to infectious disease models

Collaborators

- Sham Bhat, Los Alamos National Laboratories
- Won Chang, Statistics, Penn State University
- Roman Olson, Department of Geosciences, Penn State University
- Klaus Keller, Department of Geosciences, Penn State University

Calibration with Large Spatial Data

- Basis-representation approaches (Higdon et al., 2008, and Bayarri et al., 2008) are very effective but do not extend in obvious fashion to our problem but have some shortcomings
- Higdon et al.(JASA, 2008): May become computationally expensive if number of parameter settings and/or required number of principal components are too large (requires inversion of $(J_y + J_d) + p(J_y)$ matrix) where $J_y =$ number of principal components, $J_d =$ number of kernel basis.
- Bayarri et al. (Annals, 2007):
  - For ultra high dimensional data, their representation is not parsimonious enough.
  - Requires a dyadic(a power of 2) grid for data.

PCA-based Approach for High-dimensional Calibration

Outline of approach:

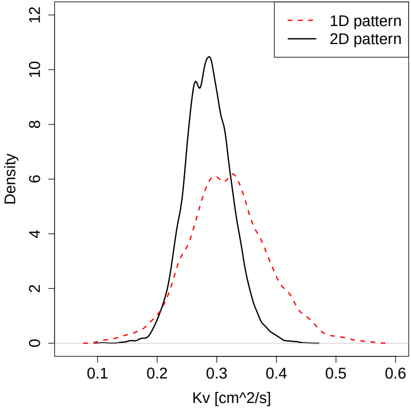
- **Dimension Reduction:** Summarize the model output $\mathbf{Y}$ and the observation $\mathbf{Z}$ using PCA and kernel basis.
  1. Find the first J_y eigenvectors $\mathbf{K}_y = (k_1, \ldots, k_{J_y})$ and the corresponding principal components $\mathbf{W}$ of the model output.
  2. Project $\mathbf{Z}$ on the space spanned by $\mathbf{K} = [\mathbf{K}_y\ \mathbf{K}_d]$ where $\mathbf{K}_d$ is the matrix of kernel basis with J_d knots. Denote the projected vector by $\mathbf{Z}_{red}$.
- **Emulation:** Construct an emulator for each of the principal components in $\mathbf{W}$ separately. Computation reduces to $\mathcal{O}((J_y + J_d)^3)$ instead of $\mathcal{O}(n^3 p^3)$. E.g. 4,913,000 flops vs 1.5×10^{16} flops.
- **Calibration:** Estimate $\boldsymbol{\theta}$ based on the likelihood function

$$|\Sigma_{\mathbf{Z}_{red}|\mathbf{W}}|^{-\frac{1}{2}} \exp[-\frac{1}{2}\mathbf{Z}_{red}^T(\Sigma_{\mathbf{Z}_{red}|\mathbf{W}} + (\mathbf{K}^T\mathbf{K})^{-1})^{-1}\mathbf{Z}_{red}.$$

PCA-based Approach for High-dimensional Calibration

Climate parameter calibration with sea temperature:

- Climate model output: 250 UVic ensembles (1D: 13, 2D: 988, 3D: 61,051 spatial points for each).
- Observation data: World Ocean Atlas 2009.



Computational Cost