On Gaussian process models for learning about climate model parameters

Murali Haran

Department of Statistics
Pennsylvania State University

(joint work with Sham Bhat (Statistics), Roman Tonkonojenkov (Geosciences) and Klaus Keller (Geosciences))

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The MOC and climate change

- The Atlantic meridional overturning circulation (MOC) carries warm upper waters into far-northern latitudes and returns cold deep waters southward across the Equator.
- Its heat transport makes a substantial contribution to the moderate climate of maritime and continental Europe (e.g. Bryden et al., 2005.)
- Any slowdown in the overturning circulation would have profound implications for climate change.

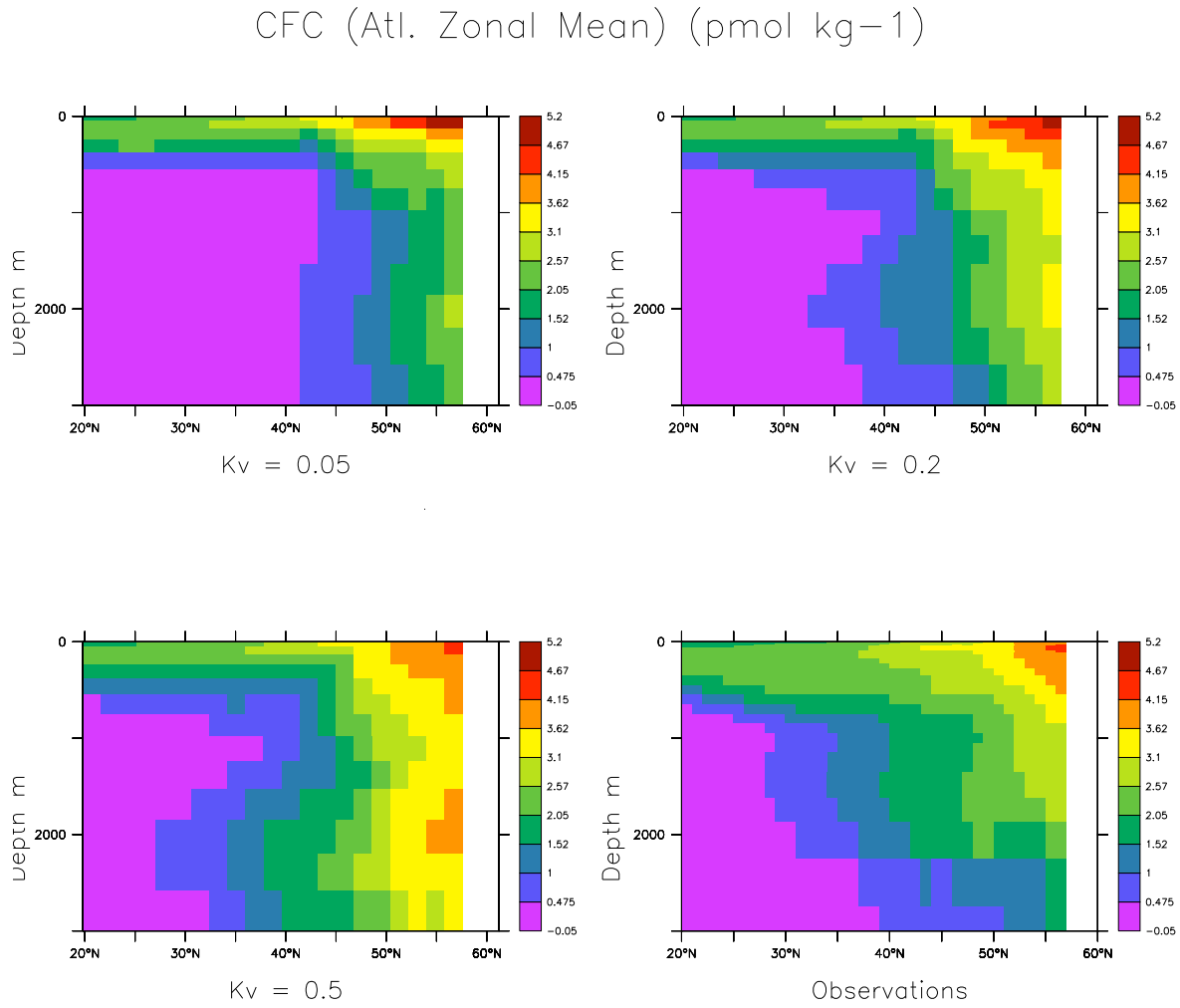
The MOC and K_v

- The potential collapse of the meridional overturning circulation (MOC) is an example of potentially catastrophic climate change.
- Climate scientists rely on sophisticated *deterministic* climate models to study such phenomena and make projections about the MOC.
- Climate models have many unknown parameters (inputs).
- A key source of uncertainty in MOC projections is uncertainty about the parameter background ocean vertical diffusivity, K_v.

Learning about K_v

- K_v is a model parameter that quantifies the intensity of vertical mixing in the ocean. Cannot be measured directly.
- We work with two sources of indirect information:
  - Observations of two ocean 'tracers', both provide information about K_v: $\Delta^{14}C$ and trichlorofluoromethane (CFC11) collected in the 1990s.
  - Climate model output at different values of K_v from the University of Victoria(UVic) Earth System Climate Model (Weaver et. al. 2001).
- Data are in the form of spatial fields.
- Data size: for each of two tracers, 3706 observations and 5926 model output per input.

CFC example

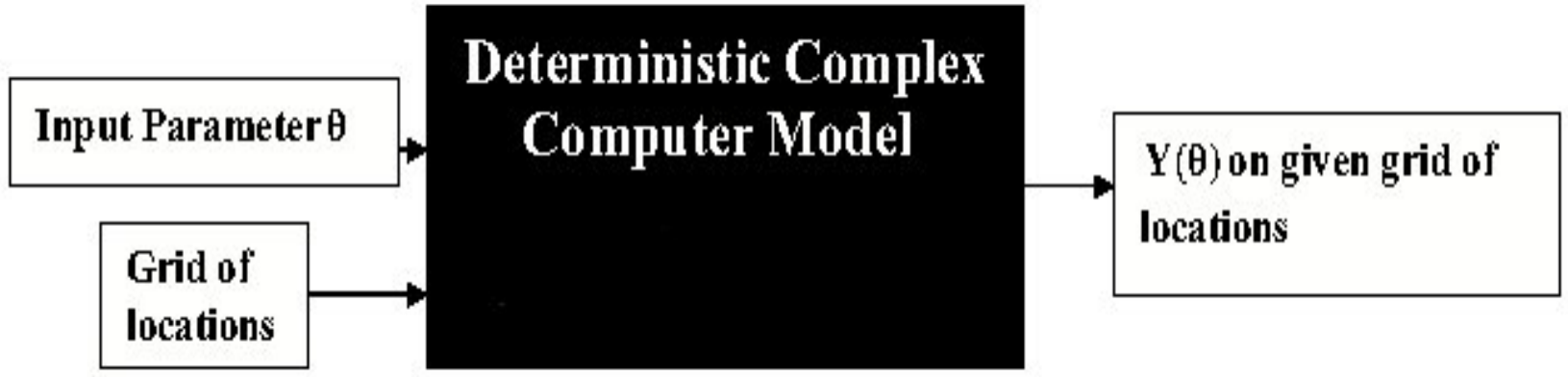


- Bottom right: observations
- Remaining plots: climate model output at 3 settings of K_v.

Challenges

1. No direct connection between observations and climate parameter. Rely on climate model runs to obtain a probability model connecting observations and climate parameter $\mathbf{K_v}$.
2. The climate model is very computationally intensive. Hence, can only be run at a few different settings.
3. Large spatial data sets: poses computational challenges for inference.
4. Combining information from multiple tracers, CFC-11, $\Delta^{14}C$: need a computationally tractable model for flexible relationships between the spatial fields.

Computer model emulation



- **Emulation** involves replacing a complicated computer model with a simpler (usually stochastic) approximation.
- Sacks et. al. (1989) introduced a linear Gaussian process model as an emulator for a complex nonlinear function. Also, Currin, Mitchell, Morris, Ylvisaker (1991), Bayarri et al (2007;2008), Sanso et al. (2008) and many others.

Gaussian processes: review

- Model random variable at location $\mathbf{s}$ by

$$Z(\mathbf{s}) = X(\mathbf{s})\beta + w(\mathbf{s}), \text{ for } \mathbf{s} \in D \subset \mathbb{R}^d$$

- $\{w(\mathbf{s}), \mathbf{s} \in D\}$ is (infinite dimensional) Gaussian process.
- Let $\mathbf{w} = (w(\mathbf{s}_1), \ldots, w(\mathbf{s}_n))^T$, $\mathbf{Z} = (Z(\mathbf{s}_1), \ldots, Z(\mathbf{s}_n))^T$.
  Predictions at new locations: $\mathbf{Z}^* = (Z(\mathbf{s}_1^*), \ldots, Z(\mathbf{s}_m^*))^T$.

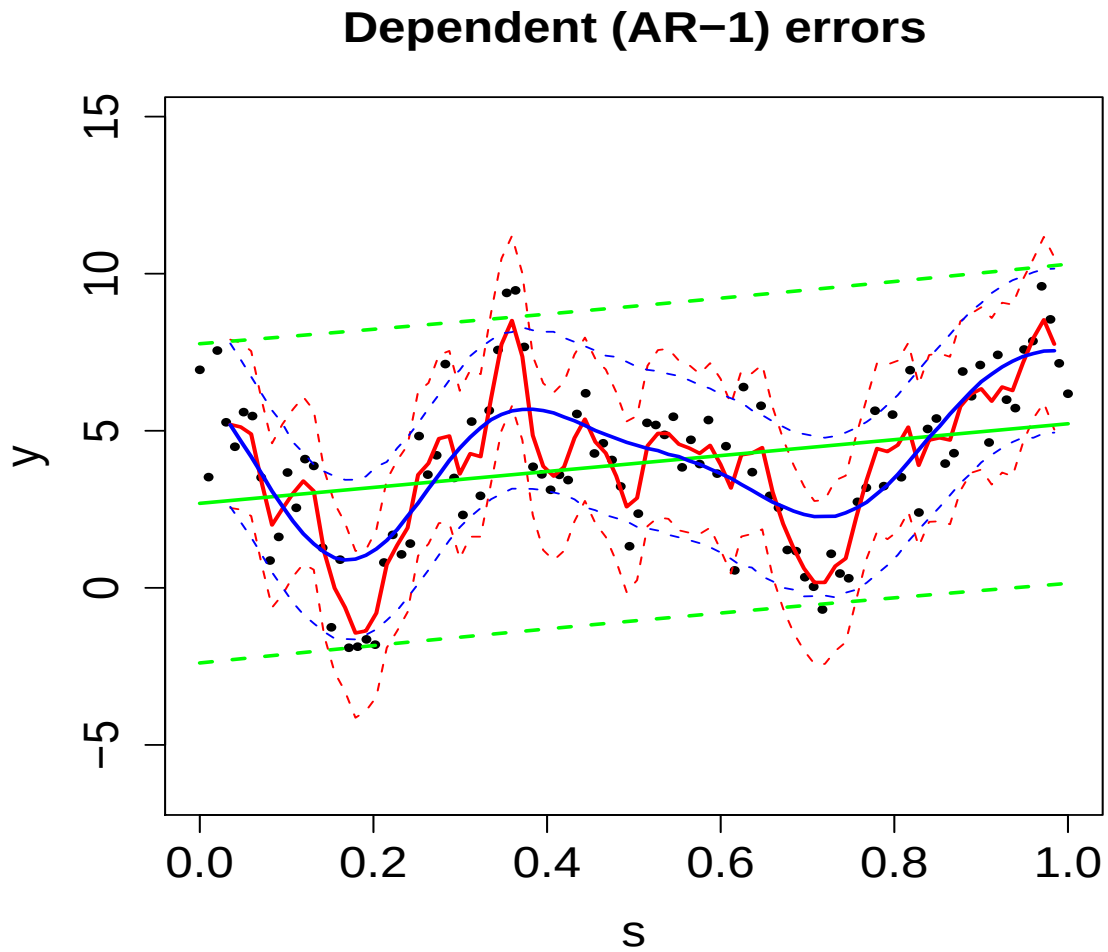
$$\mathbf{w} \mid \xi \sim N(0, \Sigma(\xi)), \quad \xi \text{ are covariance parameters}$$

- $\mathbf{Z}^* \mid \mathbf{Z}$ is normal with conditional mean, covariance:

$$E(\mathbf{Z}^* \mid \mathbf{Z}, \beta, \xi) = \mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(\mathbf{Z} - \mu_1)$$

$$\text{Cov}(\mathbf{Z}^* \mid \mathbf{Z}, \beta, \xi) = \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}.$$

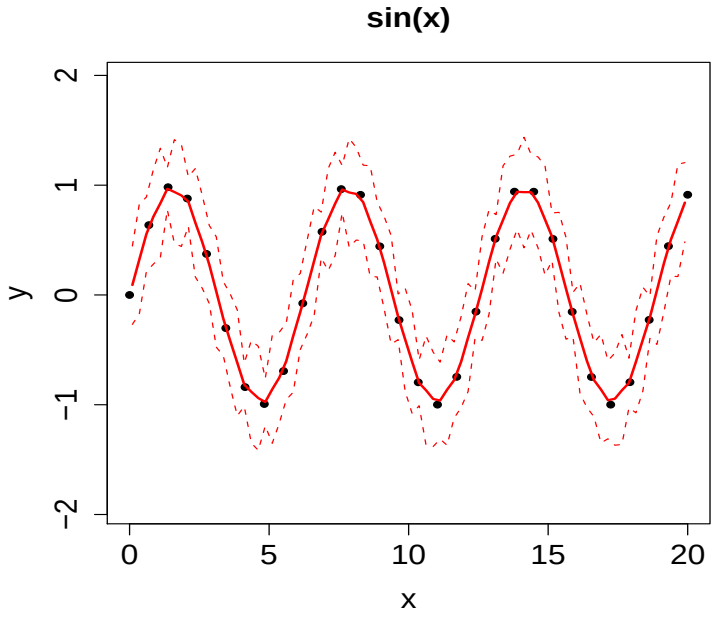
GP model for dependence: toy 1-D example

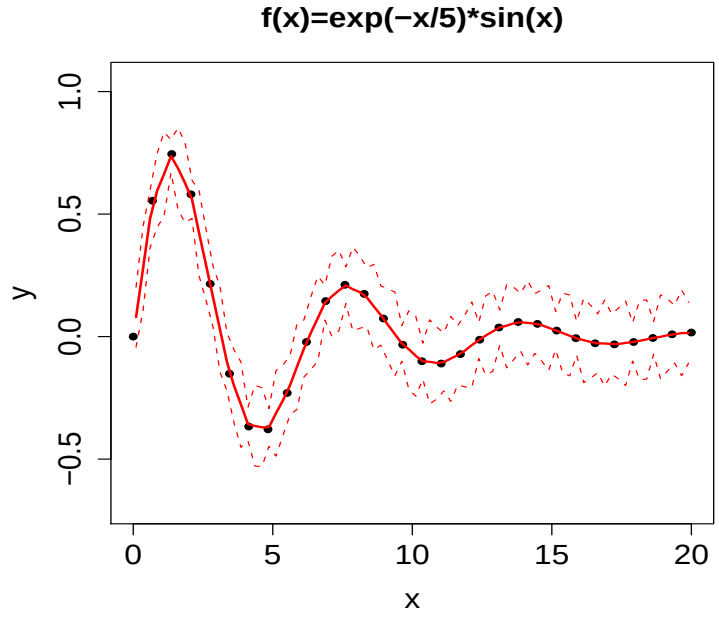


Black: 1-D AR-1 process simulation. Green: independent error.

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

GP model for emulation





Functions: $f(x) = \sin(x)$ and $f(x) = \exp(-x/5)\sin(x)$.

Both were fit with linear GP model, $f(x) = \alpha + \epsilon(x)$, where $\{\epsilon(x),\ x \in (0, 20)\}$ is a GP, α is just a constant mean.

Hence, we can use GPs for simultaneously modeling complicated functions and incorporating spatial dependence.

Notation

- $Z_1(\mathbf{s}), Z_2(\mathbf{s})$: physical observations of tracer 1 and 2 at location **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 for tracer 1 and 2 at location **s**=(latitude, depth), and climate parameter θ.
  Let $\mathbf{Y}_1, \mathbf{Y}_2$ be the model output for the two tracers.

Goal: Inference for climate parameter $\boldsymbol{\theta}$ using $\mathbf{Z}_1, \mathbf{Z}_2, \mathbf{Y}_1, \mathbf{Y}_2$.

Bayesian computer model calibration

- Kennedy and O'Hagan (2001) developed a fully Bayes approach for computer model calibration. Sanso et al. (2008) develop a model for climate parameters.
- Assumption:

$$Z(\mathbf{s_i}) = Y(\mathbf{s_i}, \theta^*) + \epsilon_i.$$

Can think of θ^* as a fitted value (Bayarri, Berger et al. 2007).

Calibration with multiple spatial fields

Two stage approach to obtain posterior of $\boldsymbol{\theta}$:

1. Model relationship between $\mathbf{Z} = (\mathbf{Z}_1, \mathbf{Z}_2)$ and $\boldsymbol{\theta}$ via emulation of model output $\mathbf{Y} = (\mathbf{Y}_1, \mathbf{Y}_2)$.
   Emulation done via a Gaussian process model.
2. Use observations $\mathbf{Z}$ to infer $\boldsymbol{\theta}$ (parameter of interest).

Calibration 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.)

$$\mathbf{Y}_1 \mid \mathbf{Y}_2, \beta_1, \xi_1, \gamma \sim N(\mu_{\beta_1}(\boldsymbol{\theta}) + \mathbf{B}(\gamma)\mathbf{Y}_2, \Sigma_{1.2}(\xi_1))$$

$$\mathbf{Y}_2 \mid \beta_2, \xi_2 \sim N(\mu_{\beta_2}(\boldsymbol{\theta}), \Sigma_2(\xi_2))$$

- $\mathbf{B}(\gamma)$ is a matrix relating $\mathbf{Y}_1$ and $\mathbf{Y}_2$, with parameters γ.
- The covariances of the Gaussian processes depend on both $\mathbf{s}$ (spatial distance) and $\boldsymbol{\theta}$ (distance in parameter space).
- βs, ξs are regression, covariance parameters.

Very flexible relationship between $\mathbf{Y}_1$ and $\mathbf{Y}_2$.

Calibration with multiple spatial fields [cont'd]

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

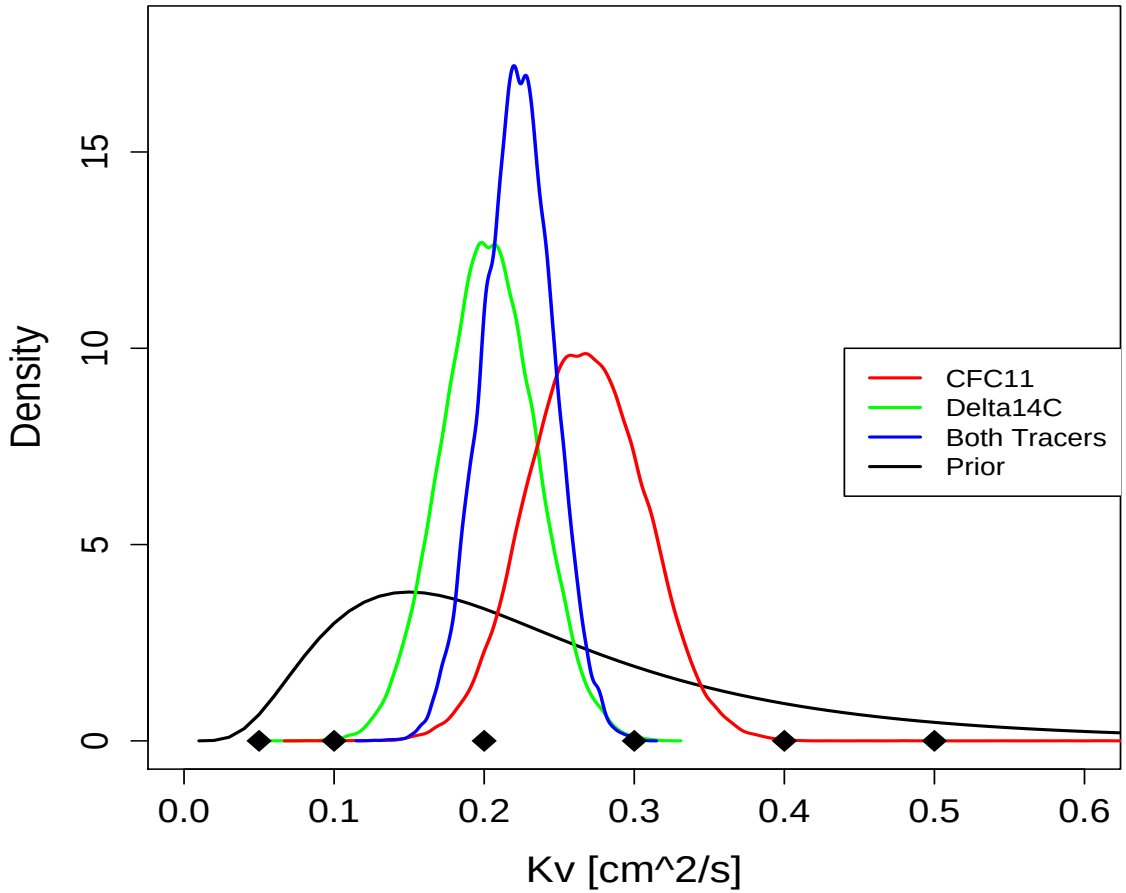
$$\mathbf{Z} = \eta(\mathbf{Y}, \boldsymbol{\theta}) + \delta(\mathbf{Y}) + \epsilon$$

  where $\delta(\mathbf{Y}) = (\delta_1\ \delta_2)^T$ is the model discrepancy, $\epsilon = (\epsilon_1\ \epsilon_2)^T$ is the observation error.
- Model discrepancy term can make crucial adjustment to $\boldsymbol{\theta}$ estimates (Bayarri et al. 2007; Bhat et al., 2010).
- Use Markov chain Monte Carlo (MCMC) to estimate $\pi(\boldsymbol{\theta} \mid \mathbf{Z}, \mathbf{Y})$, integrating 'out' remaining parameters.
- Separating stages: 'modularization' (e.g. Liu et al., 2009).

Computational issues

- Matrix computations are $\mathcal{O}(N^3)$, where N is the number of observations. Naive approach: N is in tens of thousands.
- Need long MCMC runs since there may be multimodality issues, and the chain mixes slowly.
- We use reduced rank approach based on kernel mixing (Higdon, 1998): continuous process created by convolving a discrete white noise process with a kernel function.
- Special structure + Sherman-Woodbury-Morrison identity used to reduce matrix computations.
- In MLE step: take advantage of structure of hierarchical model to reduce computations.

Results for K_v inference



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

Result: $\mathbf{K_v}$ pdf suggests weakening of MOC in the future.

Summary

1. Our approach is to perform inference in two stages:
   - Obtain a probability model connecting CFC-11, $\Delta^{14}C$ tracer observations to $\mathbf{K_v}$ by fitting a Gaussian process model to climate model runs.
   - Using this probability model, infer a posterior density for $\mathbf{K_v}$ from the observations.
2. We model multivariate spatial data via a flexible hierarchical structure.
3. We use kernel mixing to obtain patterned covariances, making computations tractable for large data sets.

We can use inferred $\mathbf{K_v}$ in the climate model to project the MOC.

Some references

- Kennedy, M.C. and O'Hagan, A.(2001), Bayesian calibration of computer models, *JRSS(B)*.
- Sanso, B,. Forest, C.E., Zantedeschi, D (2008) , Inferring Climate System Properties Using a Computer Model, *BA*.
- Higdon (1998) A process-convolution approach to modelling temperatures in the North Atlantic Ocean, *Envir. Ecol. Statistics*.
- Royle, J.A. and Berliner, L.M. (1999) A hierarchical approach to multivariate spatial modeling and prediction, *JABES*.
- Bhat, K.S., Haran, M., Tonkonojenkov, R., Keller, K. (2010) "Inferring likelihoods and climate system characteristics using climate models and multiple tracers."
- Bhat, K.S., Haran, M., Goes, M. (2010) "Computer model calibration with multivariate spatial output."

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Joint modeling approach: pros and cons

- Bayesian machinery and MCMC makes it relatively easy to write down a reasonable joint model.
- Modelers (especially Bayesians) often argue that having a joint model is critical. Pragmatic argument: propogation of uncertainty through the model.
- However, joint model adds computational burdens. Also leads to identifiability issues. Hence, in order to build a joint model: have to resort to unrealistic covariance assumptions and heavy spatial and temporal aggregation of both observations and model output.

Alternative: Two stage approach

- Two stage approach to obtain posterior of θ:
  - Model the **Y**'s stochastically to 'infer a likelihood', connecting θ to **Y**.
  - Model **Z** using fitted model from above, with additional errors, biases, to infer θ (along with errors, biases.)
- Model **Y** as a Gaussian process emulator, with mean a linear function of θ.

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

- ξ is the set of covariance parameters, covariance function assumed to be separable among **s**, t, and θ.
- Covariance parameters:
  - Maximum likelihood estimates by optimization.
  - Bayesian approach: obtain posterior via MCMC.

Two stage approach (cont'd)

- For location **s** at a given value of θ, we can then obtain the predictive distribution $\pi(\mathbf{Z}(\theta)^* \mid \mathbf{Y})$, multivariate normal for a *given* $\hat{\xi}, \hat{\beta}$ (MLE or posterior mean/mode). Otherwise this is not in closed form.
- This multivariate normal is our approximate probability model $\hat{\eta}$, written explicitly with mean and variance as functions of θ from conditional distribution.

$$\mathbf{Z} = \hat{\eta}(\mathbf{Z}^* \mid \theta^*, \mathbf{Y}) + \delta + \epsilon,$$

- where δ is the model error term and ϵ is observation error.
- $\epsilon \sim N(0, \psi I)$ and δ is modeled as a Gaussian process, ϵ and δ are assumed to be independent. Strong prior information for ϵ can help identify the errors.
- We can now perform inference on θ^*.

Observations

- Our approach is perhaps counter to standard Bayesian modeling philosophy: instead of a coherent joint model, we are fitting models stagewise.
- Principle: If we had a likelihood, $\mathcal{L}(\mathbf{Z}; \theta)$, we could perform inference for θ based on data $\mathbf{Z}$.
- Here: We are using climate model output ($\mathbf{Y}$) to 'infer' this likelihood and then perform standard likelihood-based inference. Intuitively: separate problems (see "Subjective likelihood" [Rappold, Lavine, Lozier, 2005.])
- Our approach can be seen as a way of 'cutting feedback' (Best et al. 2006; Rougier, 2008). Advantages:
  - Protecting emulator from a poor model of climate system.
  - Modeling emulator separately to facilitate careful evaluation of emulator. (Rougier, 2008).

More advantages

- Computational advantages allow for relaxing unreasonable assumptions, e.g. no need to assume same covariance for both spatiotemporal dependence and observation error.
- Potentially helps with identification of variance/covariance components since not all parameters are being estimated/sampled at once; parameters estimated from first stage are fixed.
- Concern: are we ignoring crucial variability in parameter estimates by not propogating it as in the Bayesian formulation? Data sets/problems considered so far: not obvious that this is the case. (Also, cannot compare results for the large multivariate spatial data since cannot fit the joint model.)

Kernel mixing for climate model output

- Extend kernel and knot process $\mathbf{z}$ to t and θ dimensions:

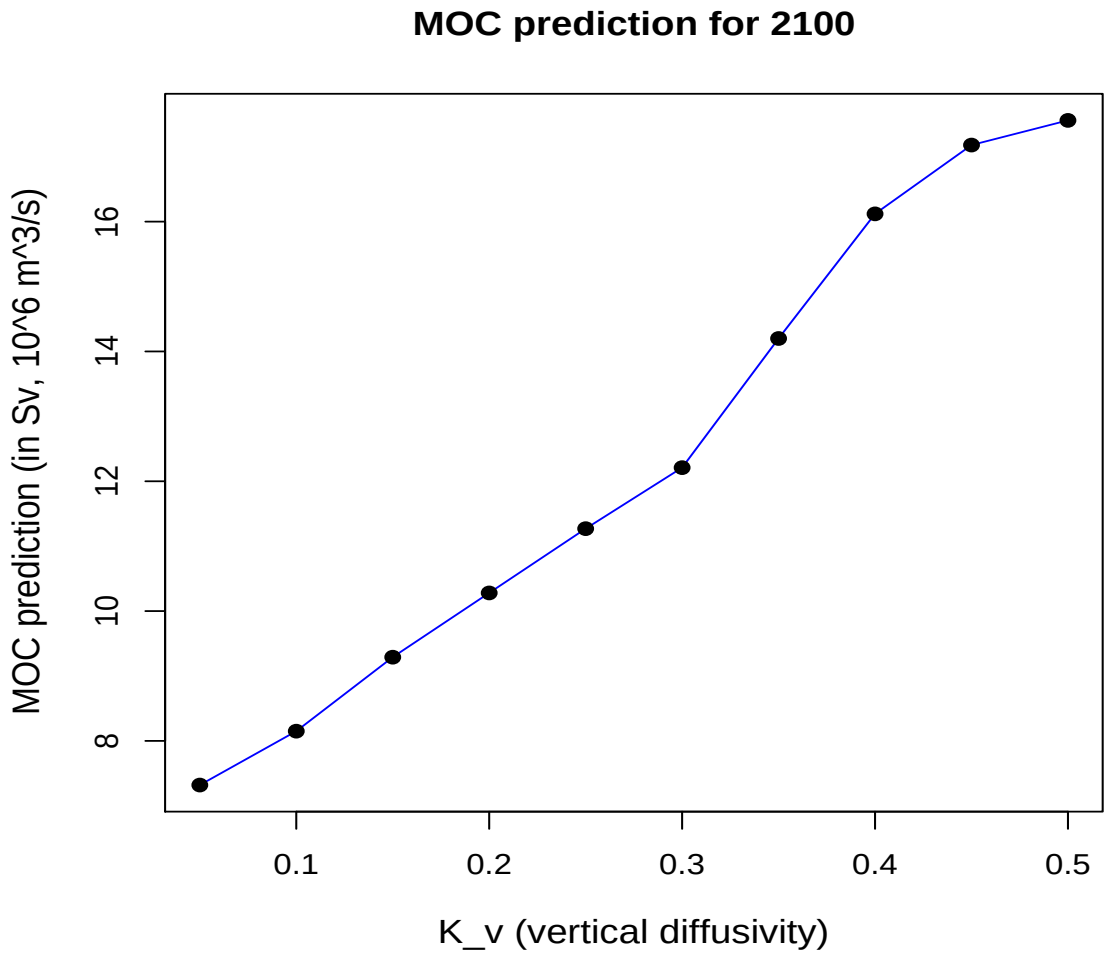
$$Y(\mathbf{s}, t, \theta) = \sum_{j=1}^{J} k(\mathbf{u}_j - \mathbf{s}; v_j - t, \ell_{1j} - \theta_1, \cdots \ell_{kj} - \theta_k) w(\mathbf{u}_j, v_j, \ell_j) + \mu(\theta)$$

- where the set of knots are $\mathbf{u}_j$, v_j, ℓ_j for $j = 1, \ldots, J$.
  $w(\mathbf{u}_j, v_j, \ell_j)$ is the process at the jth knot.
- The random field for $\mathbf{Y}(\mathbf{s}_i, t_i, \theta_i)$ is
  $\mathbf{Y}(\mathbf{s}_i, t_i, \theta_i) \mid \mathbf{w}, \psi, \kappa, \boldsymbol{\beta}, \phi_s, \phi_c$

$$\sim N\left(\mathbf{X}(\theta_i)\boldsymbol{\beta} + \sum_{j=1}^{J} K_{ij}(\phi_s, \phi_c) w(\mathbf{u}_j, v_j, \ell_j), \psi\right)$$

- Linear mean trend on θ and kernel is separable covariance function over $\mathbf{s}$, t, θ.

MOC predictions versus K_v

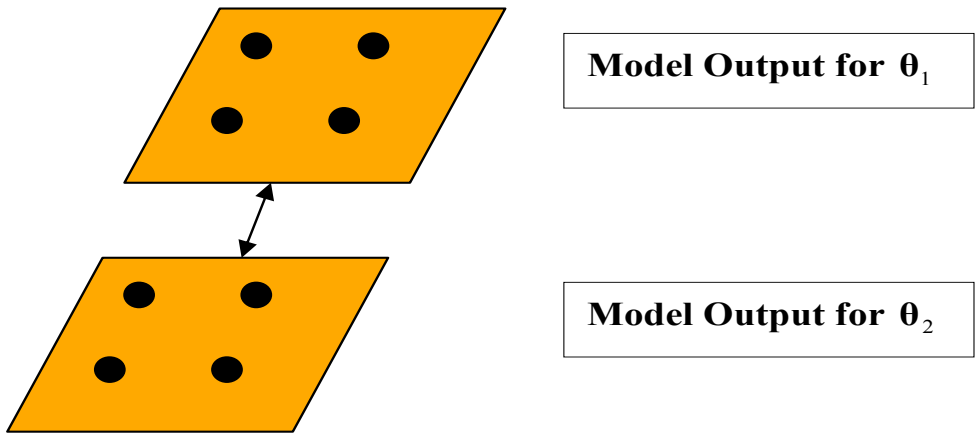


- MOC predictions are clearly much lower as K_v values get small.

Bayesian model calibration (cont'd)

- Let observation error, $\epsilon = (\epsilon_1, \cdots, \epsilon_n)^T$. Modeled as Normal $(0, \psi\Sigma)$, where Σ is estimated from other model runs (different runs from the ones used here; for e.g. 'control' runs that exclude human intervention/forcings.)
- Cov $(Y(\mathbf{s}_i, \boldsymbol{\theta}_{i'}), Y(\mathbf{s}_j, \boldsymbol{\theta}_{j'})) = \kappa\, \Sigma_{ij}\, r(\boldsymbol{\theta}_{i'}, \boldsymbol{\theta}_{j'})$.
- $\boldsymbol{\phi}_c = (\phi_{c1} \cdots \phi_{ck})$ are the climate covariance parameters.

$$r(\boldsymbol{\theta}_{i'}, \boldsymbol{\theta}_{j'}) = \prod_{m=1}^{k} \exp\left(-\frac{|\boldsymbol{\theta}_{i'm} - \boldsymbol{\theta}_{j'm}|}{\phi_{cm}}\right)$$



Bayesian model calibration: inference

- Hence the joint distribution of **Z** and **Y** is a multivariate normal, and

$$\begin{bmatrix} \mathbf{Z} \\ \mathbf{Y} \end{bmatrix} \sim N\left(\begin{bmatrix} \mathbf{M}(\boldsymbol{\theta}^*) \\ \mathbf{M} \end{bmatrix} \boldsymbol{\beta}, \begin{bmatrix} (\psi + \kappa) \otimes \Sigma & r(\boldsymbol{\theta}^*)^T \otimes \Sigma \\ r(\boldsymbol{\theta}^*) \otimes \Sigma & \mathbf{R} \otimes \Sigma \end{bmatrix} \right)$$

- Inference for $\boldsymbol{\theta}^*$, $\boldsymbol{\xi}_s$, etc is based on the posterior distribution $\pi(\boldsymbol{\theta}^*, \boldsymbol{\xi}_s, \boldsymbol{\phi}_c, \boldsymbol{\beta} | \mathbf{Z}, \mathbf{Y})$

$$\pi(\boldsymbol{\theta}^*, \boldsymbol{\xi}_s, \boldsymbol{\phi}_c, \boldsymbol{\beta} | \mathbf{Z}, \mathbf{Y}) \propto \mathcal{L}(\mathbf{Z}, \mathbf{Y} \mid \boldsymbol{\theta}^*, \boldsymbol{\xi}_s, \boldsymbol{\phi}_c, \boldsymbol{\beta}) \times p(\boldsymbol{\theta}^*) p(\boldsymbol{\xi}_s) p(\boldsymbol{\phi}_c) p(\boldsymbol{\beta})$$

  - $\mathcal{L}(\mathbf{Z}, \mathbf{Y} \mid \boldsymbol{\theta}^*, \boldsymbol{\xi}_s, \boldsymbol{\phi}_c, \boldsymbol{\beta})$: likelihood(multivariate normal)
  - $\boldsymbol{\xi}_s = (\psi, \kappa, \phi_s)$: covariance parameters.
- Priors: $\boldsymbol{\theta}^*$ based on scientific knowledge, other parameters are low precision priors (critical to do sensitivity analysis).

Computation

- $\pi(\boldsymbol{\theta}^*, \boldsymbol{\xi}_s, \phi_c, \beta | \mathbf{Z}, \mathbf{Y})$ is intractable, so rely on sample-based inference: Markov Chain Monte Carlo (MCMC).
- Computational bottleneck: matrix computations (e.g. Choleski factors) are of order N^3, where N is the number of observations.
- Kronecker products greatly reduce the computational burden. *Important*: This is brought about by assuming the same covariance Σ in modeling dependence among observations ($\mathbf{Z}$), computer model output ($\mathbf{Y}$) and in the block cross-covariance.

Kernel mixing for spatial processes

- Model spatial dependence terms ($w(\mathbf{s})$) via kernel mixing of white noise process (Higdon, 1998, 2001).
- New process created by convolving a continuous white noise process with a kernel, k, which is a circular normal.

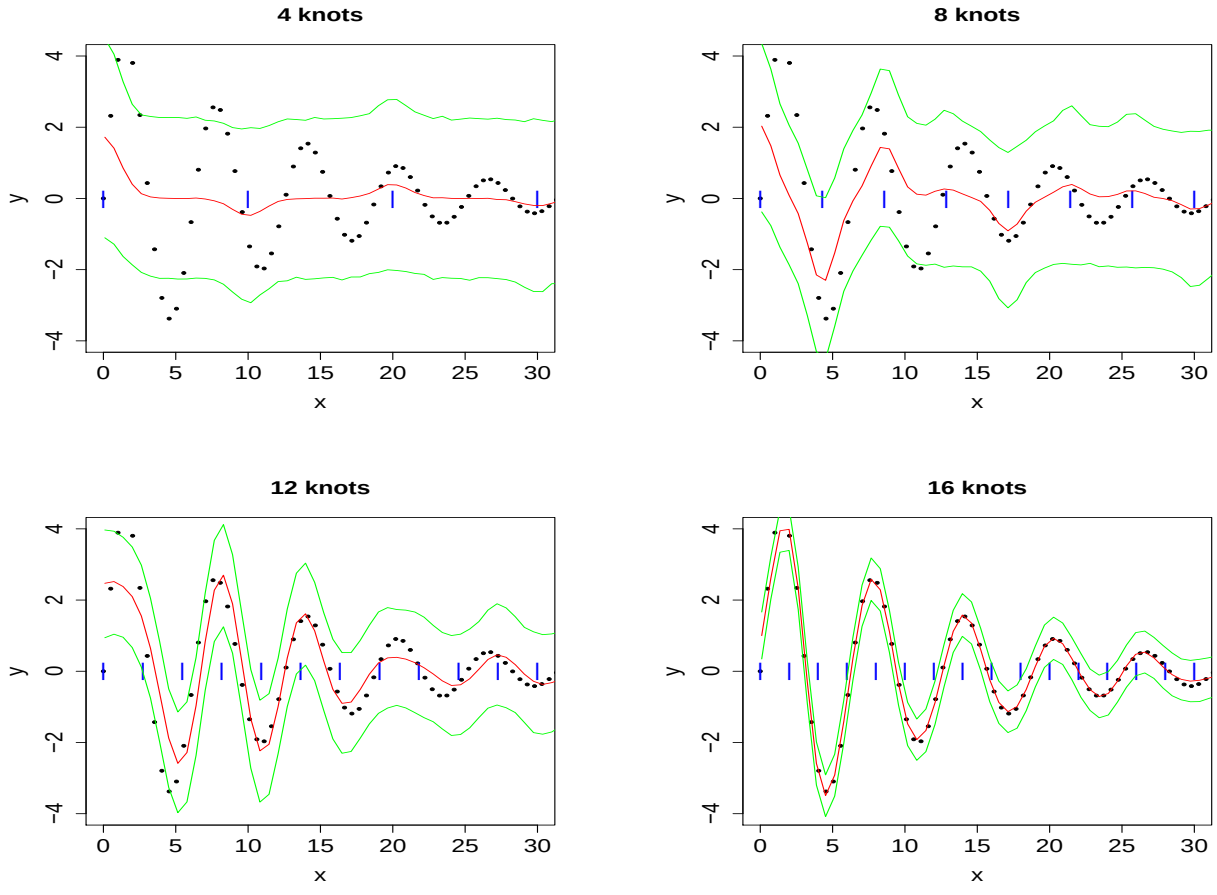
$$w(\mathbf{s}) = \int_D k(\mathbf{u} - \mathbf{s}) z(\mathbf{u}) d\mathbf{u}.$$

- Replace original GP by a finite sum approximation $\mathbf{z}$ defined on a lattice $\mathbf{u}_1, \ldots, \mathbf{u}_J$ (knot locations).

$$w(\mathbf{s}) = \sum_{j=1}^{J} k(\mathbf{u}_j - s) z(\mathbf{u}_j) + \mu(\mathbf{s}),$$

- Flexible: easily allows for non-stationarity and nonseparability. e.g. if k varies in space, have non-stationary process.

Kernel mixing for spatial processes (cont'd)



- Dimension reduction: Computation involves only the J random variables $z_1, \ldots, z_J$ at the locations $\mathbf{u}_1, \ldots, \mathbf{u}_J$.
- Figures are for 4, 8, 12, and 16 knots.

Matrix identities

- Kernel mixing can be used to induce special matrix forms that permit very fast computations. In fact, we ignore the latent variables and simply use the kernel mixing formulation to obtain matrices of special forms.
- Sherman-Woodbury-Morrison identity: Suppose a matrix can be written in the form $A + UCV$, where A is of dimension $N \times N$, U is dimension $N \times J$, V is dimension $J \times N$, and C is dimension $J \times J$. Its inverse is rewritten as:

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}.$$

This involves inversions of matrices of dimension $J \times J$ rather than $N \times N$. (our e.g. $J = 190$ versus N =4,500.)

Future work

- Many open problems, research avenues including:
  - Combining information from multiple climate models: Multiresolution/multiscale modeling ideas, Bayesian model averaging.
  - Flexible covariance functions, non-stationarity.
  - Combining information from several tracers (e.g. 5–10).
- Other projects that can potentially borrow some of this methodology:
  - Atmospheric Science: Estimating mean temperature fields over the past millenia using proxies and climate models.
  - Infectious disease: inferring infectious disease dynamics from sparse observations and dynamic models.