A Statistical Perspective on Uncertainty Quantification

Murali Haran

Department of Statistics, Pennsylvania State University

Network for Sustainable Climate Risk Management (SCRiM) Summer School, August 2014.

What This Talk is About

- I will describe why uncertainty quantification is central to climate risk management and, more broadly, to science.
- My examples will focus on the importance of uncertainty quantification when studying climate models, and particularly when climate projections are made using models.
- I will discuss some basic ideas related to statistical inference.

Uncertainty Quantification and Information

- Statistical inference provides a rigorous way to translate observations into information.
- Just as important, it provides a rigorous way to ascertain *how much* information the observations provide about the system of interest.
- Quantifying how much information there is: Central to the notion of uncertainty quantification.
- One could think of statistics as being about “solving” an inverse problem. Invariably these inverse problems (especially in climate science!) do not result in unique solutions. Noisy measurements and inaccuracies in data gathering contribute to this partially but even with perfect data, it is rare to have unique solutions.

Uncertainty Quantification and Information

- Many different solutions (solutions may be models, parameters) to the same problem. Uncertainty quantification is about thinking about the many alternatives, using the language of probability. For example, instead of: the parameter α compatible with this data is 4, say the parameter α is approximately Gamma distributed with a mean of 4 and variance of 2.
- An important issue related to uncertainty quantification is resolution.
  - Higher resolution models: may be more computationally expensive to run; physics may not be well modeled.
  - Higher resolution observation more expensive to obtain.
  - Not clear if models have skill at high resolution.

Statistical methods may be helpful to understand above.

Our Research Group

SCRiM Group: Interface of Earth System Analysis and Uncertainty Quantification

- Faculty: Chris Forest, Murali Haran, Klaus Keller, David Pollard
- Research associates/postdocs: Patrick Applegate, Rob Nicholas, Roman Olson
- Graduate students: Saksham Chandra, Won Chang, Yawen Guan, Josh Magerman
- Undergraduate students: Evan Bittner, Kira White

Climate Change and Risk

Polder dyke, Netherlands (from John Elk III, lonelyplanet.com)

Risk

- We need probability/statistics to define and quantify risk.
- Risk associated with an action = expected cost (or “loss”) for that action, “expected” = weighted average
  - Sum over { probability of outcome $\times$ cost of that outcome}
- For a particular policy, example of outcomes:
  - strength of the Atlantic Meridional overturning circulation or “AMOC”: weakening? stable?
  - global sea level rise: 2 metres? more? less ?
- To study economic impacts: relate outcome to impact. Example: sea level rise of x metres will cost \$$y$.
- Common to misunderstand and confuse probability and risk. E.g. low probability-high impact events are thought of as being more "likely" than low probability-low impact events.

Learning about Risk

- What is probability of sea level rise of 2m. in 2100 if:
  (A) Carbon emissions grow at same rate (“business as usual”)
  (B) Carbon emissions are controlled by a policy
- Of particular interest: low probability-high impact events. For example sea elvel rise of 2 metres may be a relatively low probability event but extremely expensive. "Tails" of probability distributions are important.

How do we learn about the probability of each outcome while accounting for uncertainties?

Learning about Risk through Statistical Methods

Risk assessment based on climate projections involves:

(1) Combining information from climate models and observations.

(2) Uncertainty quantification: for honest assessment of risk, critical to incorporate information about how certain or uncertain we are about various aspects of the climate projections.

(3) Addressing technical challenges related to the size of the data sets involved.

Novel statistical methods have been/are being developed to address the above issues.

What Do We Mean by “Uncertainties?”

Types of uncertainty:

(1) Aleatoric: stochasticity (randomness) in the universe. Example: if we knew a coin was fair, still would not know if a particular toss would yield heads or tails.

(2) Epistemic: uncertainty regarding our knowledge. Example: the weight of a particular coin (nickel/5c) is fixed but our knowledge about the weight is uncertain. If we knew the weights of 20 other coins (nickel/5c), we could make a better guess (reduced uncertainty).

Statistical models may be used to account for both.

Varieties of Uncertainty

One way to classify uncertainties relevant to climate policy is as follows (cf. Smith and Stern, 2011). These uncertainties are not mutually exclusive.

- Imprecision (Knightian risk): related to outcomes which we do not know precisely, but for which we believe robust, decision-relevant probability statements can be provided. E.g. uncertainty in a weather forecast
- Ambiguity (Knightian uncertainty): related to outcomes (known, unknown or disputed), for which it is difficult to make probability statements. Sometimes "scenario uncertainty" or uncertainty in an estimated probability ("second-order uncertainty").
- Intractability: related to inability to formulate or execute relevant computations

Climate Model Uncertainties

- Model projections are uncertain as models can never fully describe the climate system.
- Boundary or initial condition uncertainty.
- “Forcings” uncertainty, e.g. uncertainty about emissions.
- Observations may have measurement errors, may not be available everywhere (interpolation uncertainty).
- **Parameter uncertainty**: parameters (“dials” in the computer model) may be uncertain. The value of the parameter may affect climate projections.

Quantifying Uncertainty

- Uncertainty is not the same as not knowing.
- A lack of certainty is not a reason to avoid action. Risk may be estimated in the face of uncertainty.
- Describing uncertainties carefully is central to the scientific enterprise. For instance, “Without uncertainty quantification, it is easy to dismiss climate (computer) models.” – A. O’Hagan.

Statistical Approach for UQ: Modeling

An approach to formalize the statistical methodology used:

(1) Modeling of the system:
   - If possible, establish a forward model that describes the dynamics (physics) of the system of interest. This is a *mathematical model*, which may be implemented through computer code.
   - Add potential errors, biases to the above to account for various uncertainties. This now describes a *statistical* model for the system.
   - Denote observations of this system by **Z**, parameters of the forward model by $\boldsymbol{\theta}$, statistical parameters by ξ.
   - A "realization" (a particular instance) of **Z** is then obtained from this probability distribution, $f(\mathbf{Z}; \boldsymbol{\theta}, \boldsymbol{\xi})$

(Modulo computational challenges) it should now be possible to simulate **Z** using various values of $\boldsymbol{\theta}, \boldsymbol{\xi}$.

Statistical Approach for UQ: Inference

(2) Likelihood-based inference: General approach to take an observation of **Z** and model above and (i) estimate $\boldsymbol{\theta}, \xi$, (ii) approximate uncertainty about $\boldsymbol{\theta}, \xi$.

- Likelihood function, $\mathcal{L}(\boldsymbol{\theta}, \xi) \propto f(\mathbf{Z}; \boldsymbol{\theta}, \xi)$ with **Z** fixed at observed values. $\mathcal{L}(\boldsymbol{\theta}, \xi)$ function of *only* parameters.
- Maximize $\mathcal{L}(\boldsymbol{\theta}, \xi)$ w.r.t. $\boldsymbol{\theta}, \xi$ to obtain maximum likelihood estimates, $\hat{\boldsymbol{\theta}}, \hat{\xi}$
- Curvature of $\mathcal{L}(\boldsymbol{\theta}, \xi)$ at $\hat{\boldsymbol{\theta}}, \hat{\xi}$ approximates uncertainties. (Argument is asymptotic, i.e., as sample size tends to infinity.)
- Alternative approach: Bayesian inference.

Statistical Approach for UQ: Inference

(2*) Bayesian inference:

- Begin by specifying prior distribution for $\boldsymbol{\theta}, \xi$: What we thought they were before observing **Z**, described as a distribution, $p(\boldsymbol{\theta}, \xi)$.
- What we know about $(\boldsymbol{\theta}, \xi)$ is described by posterior distribution, $\pi(\boldsymbol{\theta}, \xi \mid \mathbf{Z}) \propto \mathcal{L}(\boldsymbol{\theta}, \xi) p(\boldsymbol{\theta}, \xi)$.
- Instead of optimization, computation is now Monte Carlo integration using Markov chain Monte Carlo (MCMC):
  - Simulate from the distribution $\pi(\boldsymbol{\theta}, \xi \mid \mathbf{Z})$.
  - Based on these simulations, approximate properties of this distribution.

Model Building and Evaluation

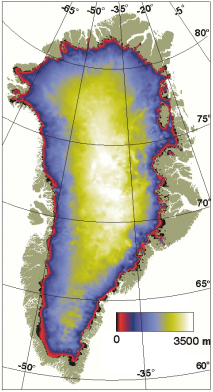
- Important: Steps 1 (Model Specification) and Step 2 (Statistical Inference) are not simply done once.
- After statistical inference/model fitting (Step 2), need to return to Step 1 to evaluate whether fitted model, error structures etc. are appropriate.
- Step 1 is difficult and important, uses both scientific and statistical expertise. May have to iterate many times before reasonable model and inference obtained.

Bayesian Framework

- Lots of arguments about foundations, theory, philosophy, both for and against Bayesian inference.
- Some practical arguments in favor of Bayes in climate:
  - Often need to build models linking multiple data sets. Inference in such cases is generally simpler with Bayes.
  - More easily learn about relationships between parameters of interest, can "integrate out" nuisance parameters and examine important parameters marginally.
  - Natural framework to incorporate scientific knowledge; particularly important in ill-posed inverse problems.

Greenland Ice Sheet

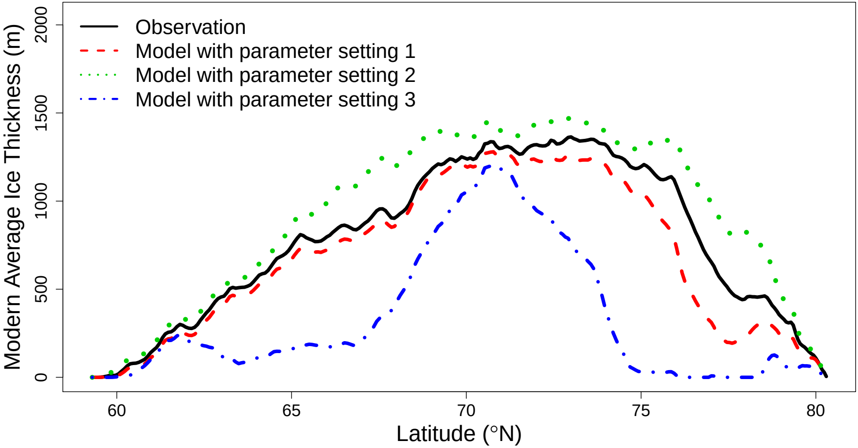
Important contributor to sea level rise: Total melting results in sea level rise of 7m.



Bamber et al. (2001)

Calibration Problem

Which parameter settings best match observations?



A Statistical Challenge in Climate Science

Focus here on one important challenge:

- Characterizing values for unknown or uncertain parameters (θ) of a climate model is called **calibration.**
- Informally: done by comparing climate model output (for various parameter values) to observations.
- Statistical model in two stages:
  1. Build an "emulator", $\eta(\theta)$ that captures relationship between θ and model output at θ, including for θ values at which model runs are not available
  2. Relate observations Z to the parameters $Z = \eta(\theta^*) + \delta(\theta^*) + \epsilon$, where δ is model-data discrepancy, ϵ is measurement error, θ^* is "fitted value" of parameter
- Can study δ and ϵ, sources of uncertainty
- Observations, model runs in the form of large spatial data

Statistical Methods

A Bayesian approach is useful:

- **Prior distribution** plausibility of various parameter (θ) values: distribution $p(\theta)$
- **Probability model** (built using climate model runs) connects parameters to observations, accounting for model-data discrepancy.
- **Posterior distribution** plausibility of various values of the parameters *given* the data, integrating all the information and sources of uncertainty

Summary: Statistical models (Gaussian processes), data reduction (principal components), matrix theory (patterned covariances), inferential algorithms (Markov chain Monte Carlo)

Computing for Bayesian Inference

1. Statistical model is fit to $\mathbf{Y} = (Y(\theta_1), \ldots, Y(\theta_p))$.
   - Maximum likelihood: optimize parameters (ξ) of Gaussian process model likelihood function, $\mathcal{L}(\mathbf{Y}; \xi)$. Result: $\hat{\xi}$
2. Denote observations by Z. Obtain a probability model from above + discrepancy. Result: likelihood $\mathcal{L}_{\hat{\xi}}(\mathbf{Z}; \theta, \gamma)$
   - θ: calibration parameters, γ: discrepancy parameters
   - Bayesian inference based on posterior distribution, $\pi(\theta \mid \mathbf{Z}) \propto \mathcal{L}_{\hat{\xi}}(\mathbf{Z}; \theta, \gamma) p(\theta, \gamma)$,
   - Above conditional distribution contains all information about θ, γ, incorporating uncertainties
   - Markov chain Monte Carlo methods: sampling approach used to learn about complicated distribution $\pi(\theta, \gamma \mid \mathbf{Z})$.
   - Learn about climate model parameters θ and discrepancy.

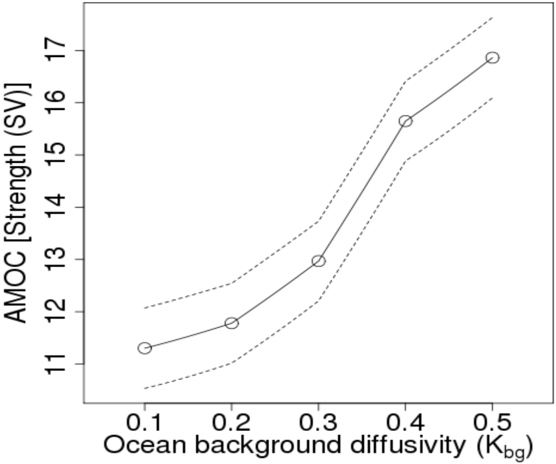
The AMOC and Climate Change

One concrete example:

- Atlantic Meridional Overturning Circulation (AMOC): AMOC heat transport makes a substantial contribution to the moderate climate of Europe (cf. Bryden et al., 2005)
- Any slowdown in the overturning circulation may have major implications for climate change
- AMOC projections from climate models.

A major source of uncertainty about the AMOC is due to uncertainty about $\mathbf{K_{bg}}$: model parameter that quantifies the intensity of vertical mixing in the ocean.

AMOC and Model Parameter K_{bg}

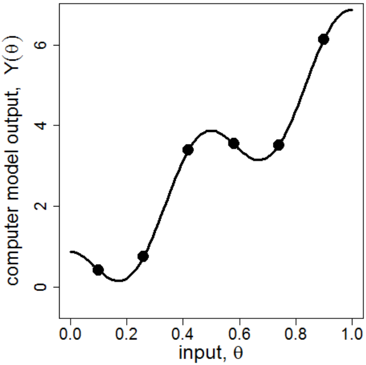


Learning about $\mathbf{K_{bg}}$

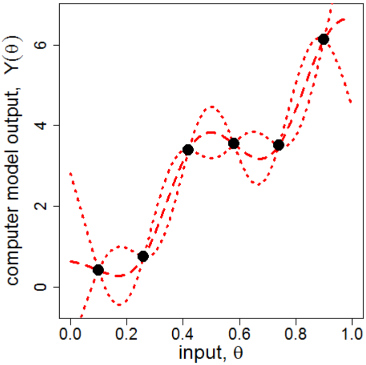
- Two sources of indirect information:
  - **Observations** of ocean temperatures.
  - **Climate model output** at different values of $\mathbf{K_{bg}}$ from University of Victoria (**UVic**) Earth System Climate Model (Weaver et. al., 2001).
- Models with different $\mathbf{K_{bg}}$ values result in markedly different ocean temperatures. Comparing observations to model output allows us to learn about $\mathbf{K_{bg}}$.

Emulation Step: A Simple Example

We use a statistical model called a **Gaussian process.** This model is a fast emulator (approximation) of the computer model.



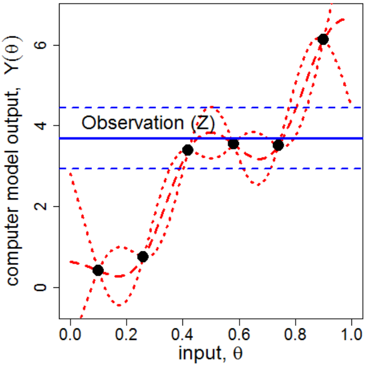
Computer model output (y-axis) vs. input (x-axis)



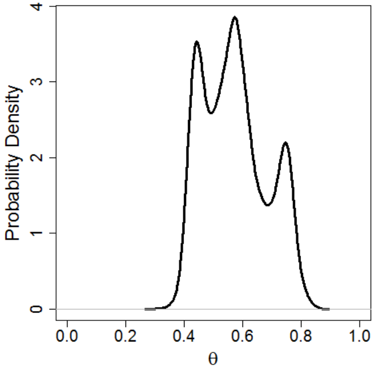
Emulation (approximation) of computer model using GP

Calibration Step: A Simple Example

We use statistical methods called **Bayesian inference and Markov chain Monte Carlo**: Use emulator (from before) and observations to learn about parameters.



Combining observation and emulator



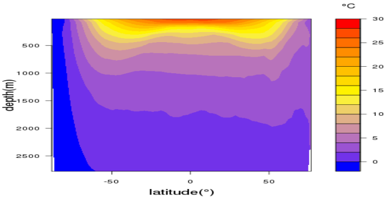
Posterior PDF of θ given model output and observation

Computational/technical challenges

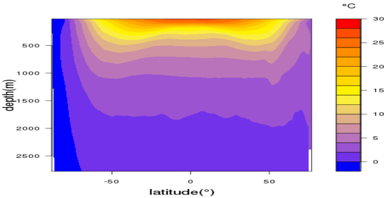
- We have 3D spatial observations and climate model output.
- Using rigorous statistical methods can be prohibitively expensive for such data. Previous methods rely on aggregation. The effect of aggregation on uncertainties is not well understood.
- Our contributions:
  1. New statistical methods and algorithms that allow us to work with the entire 3D data set without relying on aggregation.
  2. Comparison of results with unaggregated versus aggregated data: we can reduce uncertainties by using unaggregated data.

Ocean Temperatures

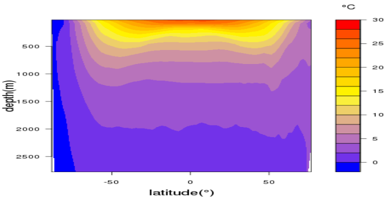
K_{bg} of 0.1



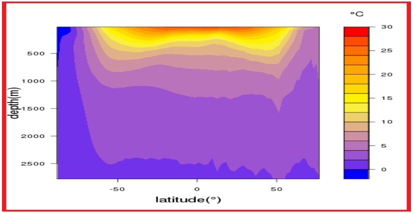
K_{bg} of 0.2



K_{bg} of 0.3

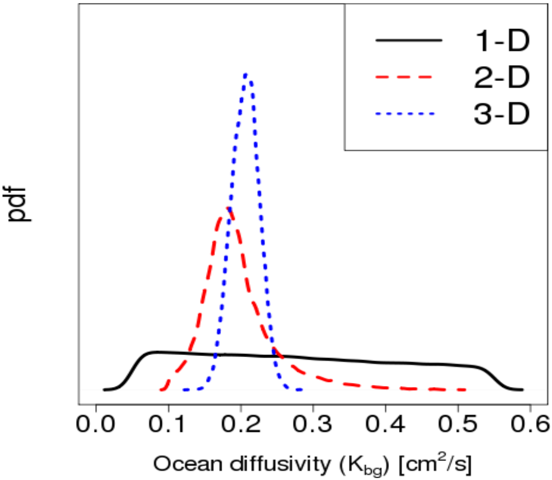


Observations



(2D versions of 3D data)

Results for $\mathbf{K_{bg}}$ Inference



(from Chang, Haran, Olson and Keller, 2013)

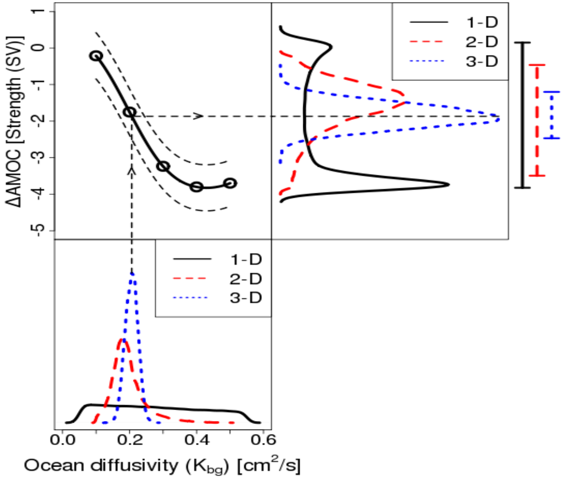
Results for $\mathbf{K_{bg}}$ Inference: Conclusions

- Our computationally efficient methods allow us to compare results from using aggregated (1D versus 2D) versus unaggregated (3D) data. Clear value:
  - Sharpest inference is based on unaggregated (3D) data.
  - Inference with 3D data is also robust to varying prior information; not so robust when using 2D or 1D data.
  - This results in sharper and more robust projections . . .
  - This is an example where UQ helps us answer questions related to the value of the resolution of models and observations.

Chang, Haran, Olson, Keller (2014, Annals of Applied Stats)

Related `R package` called stilt with simpler formulation

MOC Projections for 2100 Using Inferred K_{bg}



(from Chang, Haran, Olson and Keller, 2013)

Concluding Thoughts

- Without probability and statistics, it is not possible to quantify risk. Uncertainty quantification is central for science and policy
- General statistical tools we have developed: useful for projections of the AMOC using unaggregated data and *reduced* uncertainties. Ongoing: Greenland ice sheet volume projections.
- We can study model-data discrepancies (structural uncertainties): a term in the statistics model
- We can also learn about (complicated) interactions among model parameters.

Open Questions and Ongoing Research

- Usual caveats apply, e.g. about error structure assumptions, the fact that we are using one data set and one model; not all uncertainties are accounted for.
- We are working on several other statistical challenges in climate change risk. Examples:
  - calibration methods for non-Gaussian “zero-inflated” data
  - local impacts
  - utilizing multiple models for projections
  - using long time series tide gauge data to estimate the probability of extreme storm surges
  - estimating long term ice thinning rates in Antarctica from cosmogenic exposure dates

Collaborators

- Won Chang, Statistics, Penn State University
- Roman Olson, Earth and Environmental Systems Institute (EESI), Penn State University
- Klaus Keller, Geosciences, Penn State University
- Patrick Applegate, EESI, Penn State University

Research support from the National Science Foundation Network for Sustainable Climate Risk Management (SCRiM)

With thanks to Rob Nicholas, EESI, Chris Forest, Meteorology.

Relevant Manuscripts

- Chang, W., M. Haran, R. Olson, and K. Keller (2013): Fast dimension-reduced climate model calibration, *Annals of Applied Statistics (accepted)*
- Chang, W., Haran, M., Olson, R., and Keller, K. (2013) A composite likelihood approach to computer model calibration with high-dimensional spatial data, *Statistica Sinica (accepted)*
- Chang, W., Applegate, P., Haran, M. and Keller, K. (2013) Probabilistic calibration of a Greenland Ice Sheet model using spatially-resolved synthetic observations: toward projections of ice mass loss with uncertainties
- Olson, R., R. Sriver, M. Haran, W. Chang, N. M. Urban, and K. Keller (2013): What is the effect of unresolved internal climate variability on climate sensitivity estimates? *Journal of Geophysical Research, 118*