Introduction and overview

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Special Course on Inverse Problems
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General info about the course

- BM20A7700 Special Course on Inverse Problems.
- Lecturers: Felipe Uribe.
- M.Sc./Ph.D. Course (5 credits).
- 7 weeks; 11.01–23.02 (2024).
- Methodology: Slides and written derivations on whiteboard. Python exercises and tutorials.
- Lectures: Thursdays 14:00–17:00 (3 blocks of 45 min).
  Exercises: Fridays 10:00–12:00.
  Evaluation: Mid project (35%) and final project (35%) plus oral examination (30%).

Learning objectives

- Understand 'probabilistic objects' and their usage in uncertainty quantification.
- Apply Monte Carlo methods, evaluate their accuracy, and reduce their variance.
- Represent random variables that take values in a function space (e.g., Karhunen-Loéve expansion and neural networks).
- Apply statistical approaches to solve inverse problems (e.g., frequentist and Bayesian inference).
- Formulate different types of priors models (e.g., conjugate and hierarchical priors).
- Implement standard numerical methods for Bayesian computations (e.g., MCMC).

Lecture's schedule

– Mid project (due-date 1 week after the tutorial on week 3).
– Final project/oral exam (due-date 1 week after the tutorial on week 7).

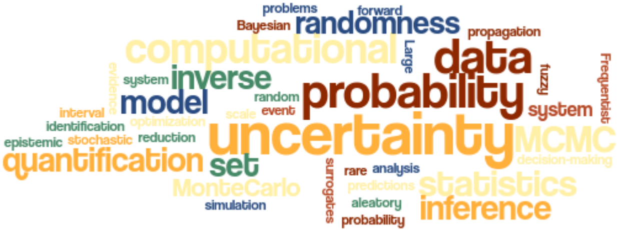
Week	Date (type)	Content
1.	11-12.01 (hybrid)	Probability theory review
2.	18-19.01 (zoom)	Monte Carlo methods and variance reduction
3.	25-26.01 (zoom)	Random fields: KLE and BNN
4.	01-02.02 (hybrid)	Intro to statistical inverse problems
5.	08-09.02 (zoom)	Prior models and intro to MCMC
6.	15-16.02 (hybrid)	MCMC
7.	22-23.02 (hybrid)	Advanced topics

The tutorial on week 3 (Friday 26) discusses the mid-term project. Unfortunately, it has to be moved to the next week; ideally Monday 29 or Tuesday 30. Let's discuss this in class.

What is in the name?

Uncertainty quantification (UQ): the science of *characterizing and reducing uncertainties* in computational models of real world phenomena.

Inverse problems (IP): consist of using the actual result of some *measurements to infer the values of parameters* that characterize a system of interest.



What is in the name?

According to the U.S. Department of Energy[1]:

"*UQ studies all sources of error and uncertainty*, including the following: systematic and stochastic measurement error; ignorance; limitations of theoretical models; limitations of numerical representations of those models; limitations of the accuracy and reliability of computations, approximations, and algorithms; and human error. A more precise definition is: UQ is the end-to-end study of the reliability of scientific inferences".

[1] U.S. Department of Energy. "Uncertainty quantification and error analysis". In: *Scientific grand challenges for national security: the role of computing at the extreme scale*. 2009, pp. 121–142.

What is in the name?

- The origins of UQ might trace back to the beginnings of the Monte Carlo method[2].
- Extended application of UQ in computational mechanics started with the seminal work[3] and the Markov chain Monte Carlo boom in the 90's.
- UQ *is not* a mature field. Both because of its youth as a field and its very close engagement with applications, UQ is much more about problems and methods. There are some very elegant approaches within UQ, but as yet no single, general theory of UQ.

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[2] N. Metropolis and S. Ulam. "The Monte Carlo Method". In: *Journal of the American Statistical Association* 44.247 (1949), pp. 335–341.

[3] R. G. Ghanem and P. D. Spanos. *Stochastic finite elements: a spectral approach*. Revised edition. Dover Publications, 2012 (Original in 1991).

UQ: definition and classification

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- **Aleatory uncertainty**: also referred to as irreducible or inherent uncertainty, is related to the natural variability of the parameters involved.
- **Epistemic uncertainty**: also known as systematic uncertainty, stems from lack of knowledge (data), therefore it can be reduced when new information is available.

There exist several theories to represent uncertainty: probability theory, fuzzy set theory, evidence theory, interval analysis, random set theory (see, e.g.,[4]).

[4] C. Joslyn and J. M. Booker. "Generalized information theory for engineering modeling and simulation". In: *Engineering Design Reliability Handbook*. Ed. by E. Nikolaidis et al. CRC Press, 2004. Chap. 9, pp. 1–40.

UQ: definition and classification

A couple of basic examples about this classification before we continue:

- **Aleatory**: *uncertainty caused by randomness*. The data-generating process of a coin flipping experiment has a stochastic nature that cannot be reduced by any source of information. A model of this process is only able to provide probabilities for the two possible outcomes (heads and tails), but no definite answer.

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- **Epistemic**: *uncertainty caused by ignorance*. What does the word 'kichwa' mean in Swahili language, head or tail? The possible answers are the same as in coin flipping, and one might be equally uncertain about which one is correct. Yet, the nature of uncertainty is different, as one could easily get rid of it.

[5] E. Hüllermeier and W. Waegeman. "Aleatoric and epistemic uncertainty in machine learning: an introduction to concepts and methods". In: *Machine Learning* 110 (2021), pp. 457–506.

Two types of UQ tasks + a bonus

In probabilistic UQ, we can distinguish the following fundamental problems:

- **Forward uncertainty propagation**: direct incorporation of the uncertain parameters through the system of interest. The main purpose is to characterize the uncertainty of the system response.
- **Inverse uncertainty quantification**: incorporation of observational data into the computational model to infer/identify the uncertain parameters describing the system of interest.
- **Model learning problem**: usage of input-ouput data to infer the computational model describing the system of interest.

Specific modeling scenarios can target several UQ objectives involving the combination of the previous tasks, e.g., *rare event simulation*, *surrogate models*, *model reduction*, *stochastic optimization*, *system identification*.

Three types of UQ tasks

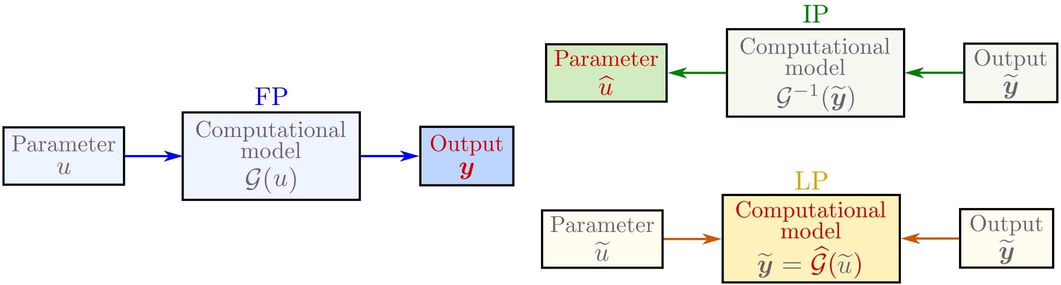


Figure: In FP, we model the uncertainty in the input and propagate it through the model to characterize the uncertainty in the output. In IP, we have data about the output which is used to naively invert the model (*don't do this*) and characterize the uncertainty in the input. In LP, we use input-output data to learn the computational model.

Some advantages in the application of (inverse) UQ

- Multiple real-life problems and phenomena are subjected to uncertainty.
- UQ can be used to assess the sensitivity of the computational model to perturbations of the governing assumptions.
- Models are imperfect (often build by approximations or discretizations), data is noisy and sparse. UQ allows us to systematically model those.
- Predictions obtained by computational models are only meaningful in the context of UQ.
- UQ supports decision-making.
- On an philosophical level: "...*It's a blessing, because it pushes us to broaden our understanding of reality and innovate*".

Some difficulties in the application of (inverse) UQ

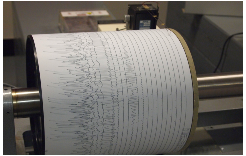
- Uncertain parameters are represented as random functions whose discretization result in high-dimensional parameter spaces (large scale problems; dimension $d > 10^4$).
- Uncertain parameters are represented as random functions with inherent discontinuities.
- The system of interest is represented with a nonlinear model.
- Evaluation of the computational model is expensive.
- Evaluation of the gradient of the computational model is prohibitive.
- On an philosophical level: "...*It's a curse, because it makes us believe and act like we known more than we actually do*".

Motivating example I: structural dynamics

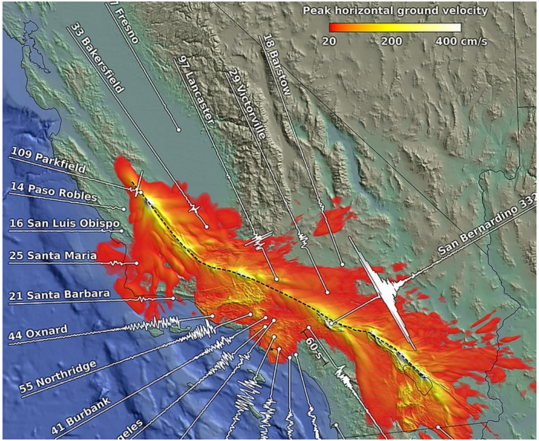
- System: the equation of motion

$$\ddot{\boldsymbol{x}}(t) + 2\xi\omega\dot{\boldsymbol{x}}(t) + \omega^2\boldsymbol{x}(t) = -\boldsymbol{a}(t).$$

- Data: recording a set of seismograms at Earth's surface.



- Inference: structural parameters ξ, ω based on the seismic acceleration $\boldsymbol{a}(t)$.



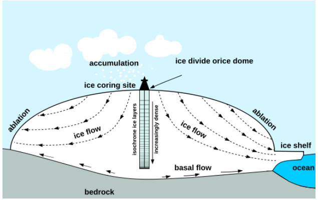
Motivating example II: ice sheet flow[6]

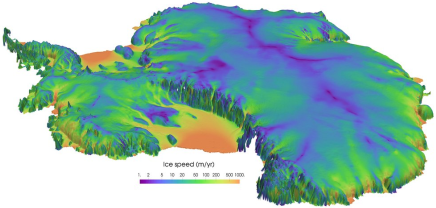
- System: nonlinear Stokes ice sheet model

$$
\begin{aligned}
-\nabla \cdot (2\eta(\boldsymbol{u})\dot{\boldsymbol{\varepsilon}}_u - \mathbf{I}\, p) = \rho\, \boldsymbol{g} \quad &\text{in } \Omega \\
\nabla \cdot \boldsymbol{u} = 0 \quad &\text{in } \Omega \\
\mathbf{T}\boldsymbol{\sigma}_u \boldsymbol{n} + \exp(\beta)\mathbf{T}\boldsymbol{u} = 0 \quad &\text{on } \Gamma
\end{aligned}
$$

- Data: current ice sheet geometry and surface ice flow velocity.

- Inference: log basal sliding coefficient β.





6 T. Isaac et al. "Scalable and efficient algorithms for the propagation of uncertainty from data through inference to prediction for large-scale problems, with application to flow of the Antarctic ice sheet". In: *Journal of Computational Physics* 296 (2015), pp. 348–368.

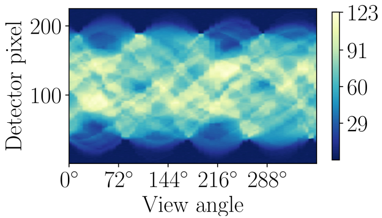
Motivating example III: X-ray computed tomography

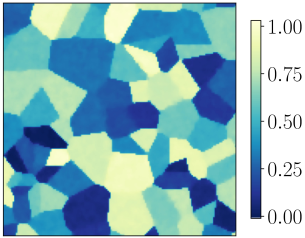
- System: Lambert–Beer's law:

$$y(\theta,\tau) = -\ln\left(\frac{I_d(\theta,\tau)}{I_s}\right) = \int_{\ell_{\theta,\tau}} x(s)\,\mathrm{d}s.$$

- Data: collection of projections $\boldsymbol{y}$ taken during the scanning process (sinogram).

- Inference: discretized attenuation coefficients $\boldsymbol{x}$.





Our target examples

In this course, we will apply UQ methods to the following one-dimensional domain applications:

- Elliptic equation.
- Signal deconvolution.

Our target examples: elliptic PDE

- We consider inference of a permeability field using observations of the pressure measured at specific locations. We define an idealized aquifer on the domain $D = [0, 1]$.

- For a given permeability $x(t, \omega)$ and source term $s(t)$, the pressure $y(t, \omega)$ follows the stochastic elliptic equation:

$$\begin{cases} \dfrac{\partial}{\partial t}\left(x(t,\omega) \dfrac{\partial y(t,\omega)}{\partial t} \right) = -s(t), & t \in D \\ x(t,\omega)\, \dfrac{\partial y}{\partial t}\Big|_{t=0} = -F(\omega), \quad y(1,\omega) = 1. \end{cases} \tag{1}$$

The permeability $x(t, \omega)$ and pressure solution $y(t, \omega)$ are random fields defined on $D \times \Omega$, where $(\Omega, \mathcal{F}, \mathbb{P})$ is a probability space.

Our target examples: elliptic PDE

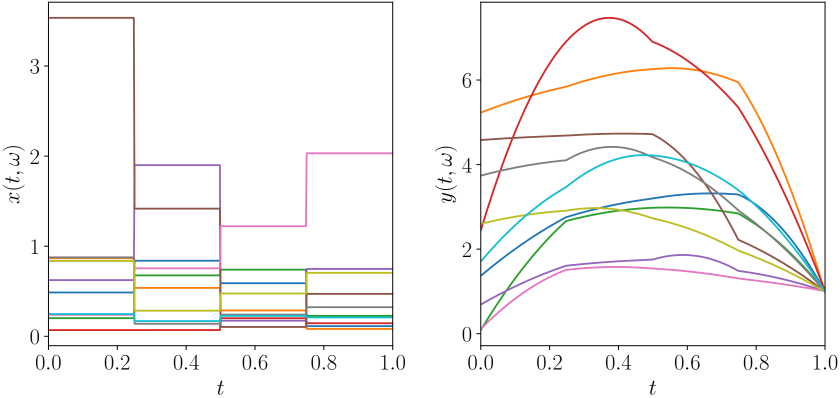


Figure: Some field realizations. Left: permeability x. Right: pressure y.

Our target examples: deconvolution

- Deconvolution is concerned with the restoration of a signal or image from a recording which is resolution limited and corrupted by noise.
- The mathematical model for convolution of a random signal on a one-dimensional spatial domain $D = [0,1]$, can be written as a stochastic Fredholm integral equation of the first kind:

$$y(t,\omega) = \int_0^1 a(t,t')x(t',\omega)\,\mathrm{d}t', \qquad t,t' \in D, \tag{2}$$

  where $x(t,\omega)$ denotes the convolved signal random variable and we assume a deterministic convolution kernel a.
- After discretizing the signal domain into N components, the convolution model can be expressed as an stochastic system of linear equations $\boldsymbol{y}(\omega) = \mathbf{A}\boldsymbol{x}(\omega)$.

Our target examples: deconvolution

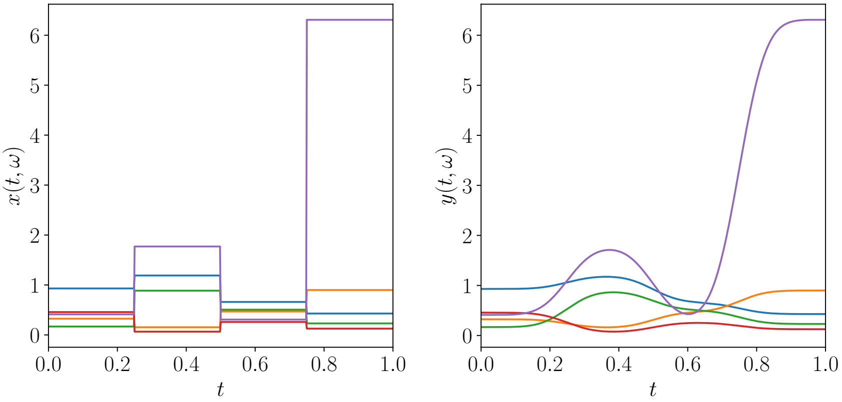


Figure: We attempt at finding the sharp signal (left), using data from a blurred signal (right).

References

[1] R. G. Ghanem et al. *Stochastic finite elements: a spectral approach*. Revised edition. Dover Publications, 2012 (Original in 1991).

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