Bayesian Inverse Problems

Jonas Latz

Input/Output: www.latz.io

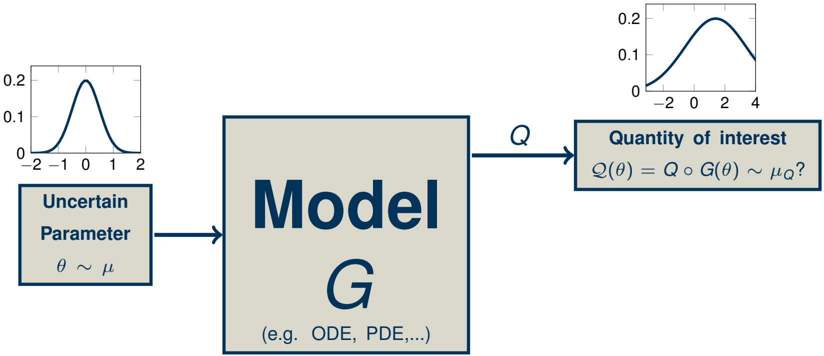
Technical University of Munich
Department of Mathematics, Chair for Numerical Analysis
Email: jonas.latz@tum.de

Garching, July 10 2018
Guest lecture in *Algorithms for Uncertainty Quantification* with Dr. Tobias Neckel and Friedrich Menhorn

Outline

Outline

Forward Problem: A Picture



Forward Problem: A few examples

Groundwater pollution.

G: Transport equation (PDE)

θ: Permeability of the groundwater reservoir

$\mathcal{Q}$: Travel time of a particle in the groundwater reservoir

Figure: Final disposal site for nuclear waste (Image: Spiegel Online)

Forward Problem: A few examples

Diabetes patient.

G: Glucose-Insulin ODE for a Diabetes-type 2 patient

θ: Model parameters such as exchange rate plasma insulin to interstitial insulin

$\mathcal{Q}$: Time to inject insulin

Figure: Glucometer (Image: Bayer AG)

Forward Problem: A few examples

Geotechnical Engineering

G: Deformation model

θ: Soil

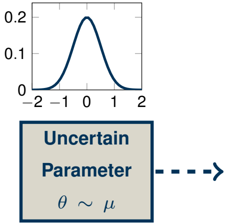
$\mathcal{Q}$: Deformation/Stability/probability of failure

Figure: Construction on Soil (Image: www.ottawaconstructionnews.com)

Distribution of the parameter θ

How do we get the distribution of θ?

Can we use data to characterise the distribution of θ?



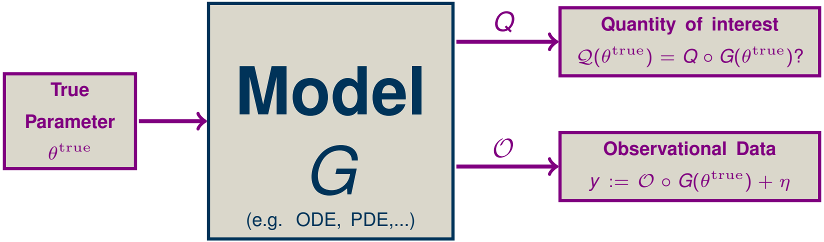
'Data'?

Let θ^{true} be the actual parameter. We define data y by

$$y := \underbrace{\mathcal{O}}_{\text{Observation operator}} \circ \overbrace{G}^{\text{Model}} (\underbrace{\theta^{\text{true}}}_{\text{actual parameter}}) + \overbrace{\eta}^{\text{measurement noise}}$$

The measurement noise is a random variable $\eta \sim \mathrm{N}(0, \Gamma)$.

‘Data’? A Picture.



Identify θ^{true}?!

Can we use the data to identify θ^{true}?

$$\Longleftrightarrow$$

Can we solve the equation $y = \mathcal{O} \circ G(\theta^{\mathrm{true}}) + \eta$?

Identify θ^{true}?!

Can we use the data to identify θ^{true}?

$$\Longleftrightarrow$$

Can we solve the equation $y = \mathcal{O} \circ G(\theta^{\mathrm{true}}) + \eta$?

Identify θ^{true}?!

Can we use the data to identify θ^{true}?

$$\iff$$

Can we solve the equation $y = \mathcal{O} \circ G(\theta^{\mathrm{true}}) + \eta$?

Identify θ^{true}?!

Can we solve equation $y = \mathcal{O} \circ G(\theta^{\text{true}}) + \eta$?

No. The problem is ill-posed.[1]

The operator $\mathcal{O} \circ G$ is very complex

$\dim(X \times Y) \gg \dim Y$, where $(X \times Y) \ni (\theta, \eta)$ and $Y \ni y$.

[1]Hadamard (1902) - *Sur les problèmes aux dérivés partielles et leur signification physique*, Princeton University Bulletin 13, pp. 49-52

Identify θ^{true}?!

Can we solve equation $y = \mathcal{O} \circ G(\theta^{\mathrm{true}}) + \eta$?

No. The problem is ill-posed.[1]

- The operator $\mathcal{O} \circ G$ is very complex
- $\dim(X \times Y) \gg \dim Y$, where $(X \times Y) \ni (\theta, \eta)$ and $Y \ni y$.

[1] Hadamard (1902) - *Sur les problèmes aux dérivés partielles et leur signification physique*, Princeton University Bulletin 13, pp. 49-52

Summary

We want to use noisy observational data y to find θ^{true}, but we cannot.

The uncertain parameter θ is still uncertain, even if we observe data y.

2 Questions:

How can we quantify the uncertainty in θ considering the data y?

How does this change the probability distribution of our Quantity of interest $\mathcal{Q}$?

We want to use noisy observational data y to find θ^{true}, but we cannot.

The uncertain parameter θ is still uncertain, even if we observe data y.

2 Questions:

How can we quantify the uncertainty in θ considering the data y?

How does this change the probability distribution of our Quantity of interest $\mathcal{Q}$?

Outline

An Experiment

We roll a die.
The sample space of this experiment is

$$\Omega := \{1, ..., 6\}.$$

The space of events is the power set of Ω:

$$\mathcal{A} := 2^{\Omega} := \{A : A \subseteq \Omega\}.$$

The probability measure is the Uniform measure on Ω:

$$\mathbb{P} := \mathrm{Unif}_{\Omega} := \sum_{\omega \in \Omega} \frac{1}{6} \delta_{\omega}.$$

An Experiment

We roll a die.

Consider the event $A := \{6\}$.

The probability of A is $\mathbb{P}(A) = 1/6$.

Now, an oracle tells us before rolling the die, whether the outcome would be even or odd.

$B := \{2, 4, 6\}$,

$B^c := \{1, 3, 5\}$.

How does the probability of A change, if we know whether B or B^c occurs?

$\rightarrow$ Conditional Probabilities

An Experiment

We roll a die.

- Consider the event $A := \{6\}$.
  - The probability of A is $\mathbb{P}(A) = 1/6$.
- Now, an oracle tells us before rolling the die, whether the outcome would be even or odd.
  - $B := \{2, 4, 6\}$,
  - $B^c := \{1, 3, 5\}$.
- How does the probability of A change, if we know whether B or B^c occurs?

$\rightarrow$ Conditional Probabilities

Conditional probabilities

Consider a probability space $(\Omega, \mathcal{A}, \mathbb{P})$ and two events $D_1, D_2 \in \mathcal{A}$, such that $\mathbb{P}(D_2) > 0$.
The conditional probability distribution of D_1 given the event D_2 is defined by:

$$\mathbb{P}(D_1|D_2) := \frac{\mathbb{P}(D_1 \text{ and } D_2)}{\mathbb{P}(D_2)} := \frac{\mathbb{P}(D_1 \cap D_2)}{\mathbb{P}(D_2)}$$

Conditional probabilities: Moving back to the experiment.

We roll a die.

$$\mathbb{P}(A|B) = \frac{\mathbb{P}(\{6\})}{\mathbb{P}(\{2,4,6\})} = \frac{1/6}{1/2} = \frac{1}{3},$$

$$\mathbb{P}(A|B^c) = \frac{\mathbb{P}(\emptyset)}{\mathbb{P}(\{1,3,5\})} = \frac{0}{1/2} = 0.$$

Probability distributions can be used to model knowledge.

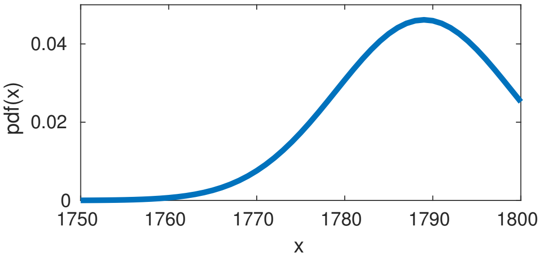
When using a fair die, we have no knowledge whatsoever concerning the outcome:

$$\mathbb{P}(\{1\}) = \mathbb{P}(\{2\}) = \mathbb{P}(\{3\}) = \mathbb{P}(\{4\}) = \mathbb{P}(\{5\}) = \mathbb{P}(\{6\}) = 1/6$$

Probability and Knowledge

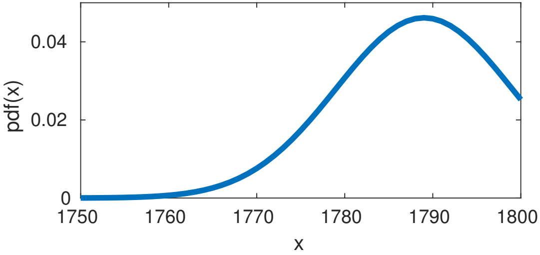
Probability distributions can be used to model knowledge.

When did the French revolution start? Rough knowledge from school: End of the 18th Century, definitely not before 1750/ after 1800.



Probability and Knowledge

Probability distributions can be used to model knowledge.



Here, the probability distribution is given by a probability density function (pdf), i.e.

$$\mathbb{P}(A) = \int_A \mathrm{pdf}(x)\mathrm{d}x$$

Conditional probability and Learning

We represent content we learn by an event $B \subseteq 2^{\Omega}$.

$$\text{Learning } B \text{ is a map } \mathbb{P}(\cdot) \mapsto \mathbb{P}(\cdot|B).$$

Conditional probability and Learning

We learn that $B = \{2, 4, 6\}$ occurs. Hence, we map

$$[\mathbb{P}(\{1\}) = \mathbb{P}(\{2\}) = \mathbb{P}(\{3\}) = \mathbb{P}(\{4\}) = \mathbb{P}(\{5\}) = \mathbb{P}(\{6\}) = 1/6]$$

$$\downarrow \qquad\qquad \downarrow$$

$$\begin{bmatrix} \mathbb{P}(\{1\}|B) = \mathbb{P}(\{3\}|B) = \mathbb{P}(\{5\}|B) = 0; \\ \mathbb{P}(\{2\}|B) = \mathbb{P}(\{4\}|B) = \mathbb{P}(\{6\}|B) = 1/3 \end{bmatrix}$$

But, how do we do this in general?

We learn that $B = \{2, 4, 6\}$ occurs. Hence, we map

$$[\mathbb{P}(\{1\}) = \mathbb{P}(\{2\}) = \mathbb{P}(\{3\}) = \mathbb{P}(\{4\}) = \mathbb{P}(\{5\}) = \mathbb{P}(\{6\}) = 1/6]$$

$$\downarrow \qquad\qquad\qquad \downarrow$$

$$\begin{bmatrix} \mathbb{P}(\{1\}|B) = \mathbb{P}(\{3\}|B) = \mathbb{P}(\{5\}|B) = 0; \\ \mathbb{P}(\{2\}|B) = \mathbb{P}(\{4\}|B) = \mathbb{P}(\{6\}|B) = 1/3 \end{bmatrix}$$

But, how do we do this in general?

Elementary Bayes' Theorem

Consider a probability space $(\Omega, \mathcal{A}, \mathbb{P})$ and two events $D_1, D_2 \in \mathcal{A}$, such that $\mathbb{P}(D_2) > 0$. Then,

$$\mathbb{P}(D_1|D_2) = \frac{\mathbb{P}(D_2|D_1)\mathbb{P}(D_1)}{\mathbb{P}(D_2)}$$

Proof: We have

$$\mathbb{P}(D_1|D_2) = \frac{\mathbb{P}(D_1 \cap D_2)}{\mathbb{P}(D_2)} \text{ (1) and } \mathbb{P}(D_2|D_1) = \frac{\mathbb{P}(D_2 \cap D_1)}{\mathbb{P}(D_1)} \text{ (2) }.$$

(2) is equivalent to $\mathbb{P}(D_2 \cap D_1) = \mathbb{P}(D_2|D_1)\mathbb{P}(D_1)$, which can be substituted into (1) to get the final result.

Elementary Bayes' Theorem

Consider a probability space $(\Omega, \mathcal{A}, \mathbb{P})$ and two events $D_1, D_2 \in \mathcal{A}$, such that $\mathbb{P}(D_2) > 0$. Then,

$$\mathbb{P}(D_1 | D_2) = \frac{\mathbb{P}(D_2 | D_1)\mathbb{P}(D_1)}{\mathbb{P}(D_2)}$$

Proof: We have

$$\mathbb{P}(D_1 | D_2) = \frac{\mathbb{P}(D_1 \cap D_2)}{\mathbb{P}(D_2)} \ (1) \text{ and } \mathbb{P}(D_2 | D_1) = \frac{\mathbb{P}(D_2 \cap D_1)}{\mathbb{P}(D_1)} \ (2) \ .$$

(2) is equivalent to $\mathbb{P}(D_2 \cap D_1) = \mathbb{P}(D_2 | D_1)\mathbb{P}(D_1)$, which can be substituted into (1) to get the final result.

Who is Bayes?

Figure: Bayes (Image: Terence O'Donnell, History of Life Insurance in Its Formative Years (Chicago: American Conservation Co:, 1936))

Thomas Bayes, 1701-1761

- English, Presbyterian Minister, Mathematician, Philosopher
- Proposed a (very) special case of Bayes' Theorem
- Not much known about him (the image above might be not him)

Who do we know Bayes’ Theorem from?

Figure: Laplace (Image: Wikipedia)

Pierre-Simon Laplace, 1749–1827

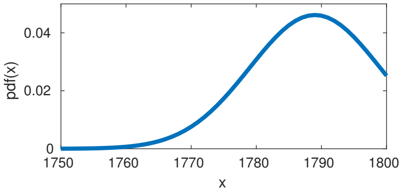
French, Mathematician and Astronomer

Published Bayes’ Theorem in ‘Théorie analytique des probabilités’ in 1812

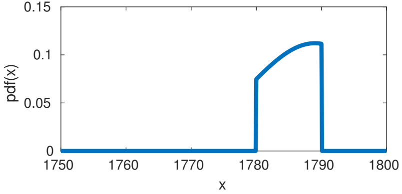
Conditional probability and Learning

When did the French revolution start?

(1) Rough knowledge from school: End of the 18th Century, definitely not before 1750/ after 1800.



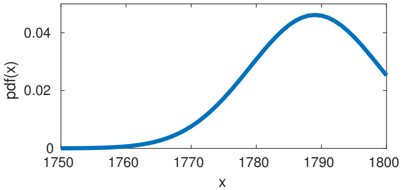
(2) Today in the radio : It was in the 1780s, so in the interval $[1780, 1790)$.



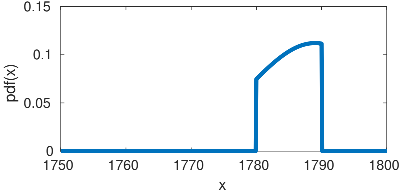
Conditional probability and Learning

When did the French revolution start?

(1) Rough knowledge from school: End of the 18th Century, definitely not before 1750/ after 1800.



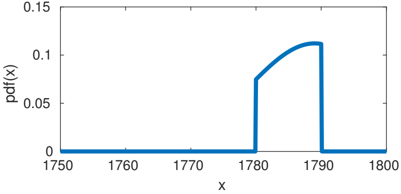
(2) Today in the radio : It was in the 1780s, so in the interval $[1780, 1790)$.



Conditional probability and Learning

When did the French revolution start?

(2) Today in the radio : It was in the 1780s, so in the interval $[1780, 1790)$.

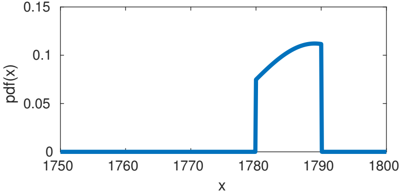


(Image: Wikipedia)

(3) Reading in a textbook: It was in the middle of year 1789.
Problem. The point in time x, we are looking for, is now set to a particular value $x = 1789.5 + \eta$, where $\eta \sim \mathrm{N}(0, 0.0625)$. Hence, the event we learn is $B = \{x + \eta = 1789.5\}$. But, $\mathbb{P}(B) = 0$. Hence $\mathbb{P}(\cdot|B)$ is not defined and Bayes' Theorem does not hold.

When did the French revolution start?

(2) Today in the radio : It was in the 1780s, so in the interval $[1780, 1790)$.



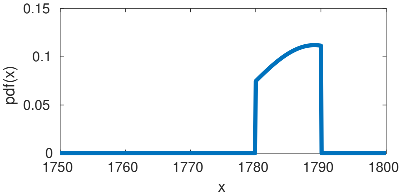
(Image: Wikipedia)

(3) Reading in a textbook: It was in the middle of year 1789.

Problem. The point in time x, we are looking for, is now set to a particular value $x = 1789.5 + \eta$, where $\eta \sim \mathrm{N}(0, 0.0625)$. Hence, the event we learn is $B = \{x + \eta = 1789.5\}$. But, $\mathbb{P}(B) = 0$. Hence $\mathbb{P}(\cdot|B)$ is not defined and Bayes' Theorem does not hold.

When did the French revolution start?

(2) Today in the radio : It was in the 1780s, so in the interval $[1780, 1790)$.



(Image: Wikipedia)

(3) Reading in a textbook: It was in the middle of year 1789.
Problem. The point in time x, we are looking for, is now set to a particular value $x = 1789.5 + \eta$, where $\eta \sim \mathrm{N}(0, 0.0625)$. Hence, the event we learn is $B = \{x + \eta = 1789.5\}$. But, $\mathbb{P}(B) = 0$. Hence $\mathbb{P}(\cdot|B)$ is not defined and Bayes' Theorem does not hold.

Non-elementary Conditional Probability

It is possible to define conditional probabilities for (non-empty) events B, with $\mathbb{P}(B) = 0$.
(rather complicated)

Easier: Consider the learning in terms of continuous random variables. (rather simple)

Conditional Densities

We learn a random variable x_1 and observe another random variable x_2

The joint distribution of x_1 and x_2 is given by a 2-dimensional probability density function $\mathrm{pdf}(x_1, x_2)$.

Given $\mathrm{pdf}(x_1, x_2)$ the marginal distributions of x_1, x_2 are given by

$$\mathrm{mpdf}_1(x_1) = \int \mathrm{pdf}(x_1, x_2)\mathrm{d}x_2; \quad \mathrm{mpdf}_2(x_2) = \int \mathrm{pdf}(x_1, x_2)\mathrm{d}x_1$$

We learn the event $B = \{x_2 = b\}$, for some $b \in \mathbb{R}$. Here, the conditional distribution is given by

$$\mathrm{cpdf}_{1|2}(x_1|x_2 = b) = \mathrm{pdf}(x_1, b)/\mathrm{mpdf}(b)$$

Bayes' Theorem for Conditional Densities

Similarly to the Elementary Bayes' Theorem, we can give a Bayes Theorem for Densities

$$\underbrace{\mathrm{cpdf}_{1|2}(\cdot|x_2 = b)}_{\text{posterior}} = \underbrace{\mathrm{cpdf}_{2|1}(b|x_1 = \cdot)}_{\text{(data) likelihood}} \underbrace{\mathrm{mpdf}_1(\cdot)}_{\text{prior}} \, / \, \underbrace{\mathrm{mpdf}_2(b)}_{\text{evidence}}$$

prior: Knowledge we have a priori concerning x_1
likelihood: The probability distribution of the data given x_1
posterior: Knowledge we have concerning x_2 knowing that $x_2 = b$
evidence: Assesses the model assumptions

Bayes' Theorem for Conditional Densities

Similarly to the Elementary Bayes' Theorem, we can give a Bayes Theorem for Densities

$$\underbrace{\mathrm{cpdf}_{1|2}(\cdot|x_2 = b)}_{\text{posterior}} = \underbrace{\mathrm{cpdf}_{2|1}(b|x_1 = \cdot)}_{\text{(data) likelihood}} \underbrace{\mathrm{mpdf}_1(\cdot)}_{\text{prior}} \,/\, \underbrace{\mathrm{mpdf}_2(b)}_{\text{evidence}}$$

prior: Knowledge we have a priori concerning x_1
likelihood: The probability distribution of the data given x_1
posterior: Knowledge we have concerning x_2 knowing that $x_2 = b$
evidence: Assesses the model assumptions

Bayes' Theorem for Conditional Densities

Similarly to the Elementary Bayes' Theorem, we can give a Bayes Theorem for Densities

$$\underbrace{\mathrm{cpdf}_{1|2}(\cdot|x_2 = b)}_{\text{posterior}} = \underbrace{\mathrm{cpdf}_{2|1}(b|x_1 = \cdot)}_{\text{(data) likelihood}}\,\underbrace{\mathrm{mpdf}_1(\cdot)}_{\text{prior}} \,/\, \underbrace{\mathrm{mpdf}_2(b)}_{\text{evidence}}$$

prior: Knowledge we have a priori concerning x_1
likelihood: The probability distribution of the data given x_1
posterior: Knowledge we have concerning x_2 knowing that $x_2 = b$
evidence: Assesses the model assumptions

Bayes' Theorem for Conditional Densities

Similarly to the Elementary Bayes' Theorem, we can give a Bayes Theorem for Densities

$$\underbrace{\mathrm{cpdf}_{1|2}(\cdot|x_2 = b)}_{\text{posterior}} = \underbrace{\mathrm{cpdf}_{2|1}(b|x_1 = \cdot)}_{\text{(data) likelihood}}\underbrace{\mathrm{mpdf}_1(\cdot)}_{\text{prior}} \,/\, \underbrace{\mathrm{mpdf}_2(b)}_{\text{evidence}}$$

prior: Knowledge we have a priori concerning x_1
likelihood: The probability distribution of the data given x_1
posterior: Knowledge we have concerning x_2 knowing that $x_2 = b$
evidence: Assesses the model assumptions

Bayes' Theorem for Conditional Densities

Similarly to the Elementary Bayes' Theorem, we can give a Bayes Theorem for Densities

$$\underbrace{\mathrm{cpdf}_{1|2}(\cdot|x_2 = b)}_{\text{posterior}} = \underbrace{\mathrm{cpdf}_{2|1}(b|x_1 = \cdot)}_{\text{(data) likelihood}} \underbrace{\mathrm{mpdf}_1(\cdot)}_{\text{prior}} / \underbrace{\mathrm{mpdf}_2(b)}_{\text{evidence}}$$

prior: Knowledge we have a priori concerning x_1
likelihood: The probability distribution of the data given x_1
posterior: Knowledge we have concerning x_2 knowing that $x_2 = b$
evidence: Assesses the model assumptions

Laplace's formulation

ce qui est le principe énoncé ci-dessus, lorsque toutes les causes sont *à priori* également possibles. Si cela n'est pas, en nommant p la probabilité *à priori* de la cause que nous venons de considérer; on aura $E = Hp$; et en suivant le raisonnement précédent, on trouvera

$$P = \frac{Hp}{S.Hp};$$

ce qui donne les probabilités des diverses causes, lorsqu'elles ne sont pas toutes, également possibles *à priori*.

Pour appliquer le principe précédent à un exemple, supposons qu'une urne renferme trois boules dont chacune ne puisse être que,

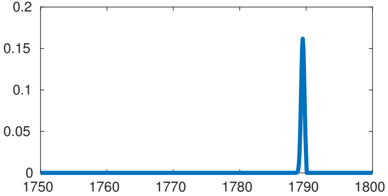
Figure: Bayes' Theorem in 'Théorie analytique des probabilités' by Pierre-Simon Laplace (1812, pp. 182)

prior p, likelihood H, posterior P, integral/sum S.

Conditional probability and Learning

When did the French revolution start?

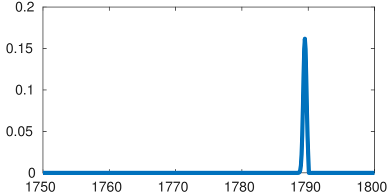
(3) Reading in a textbook: It was in the middle of year 1789.



(4) Looking it up on wikipedia.org: The actual date is 14. Juli 1789

When did the French revolution start?

(3) Reading in a textbook: It was in the middle of year 1789.



(4) Looking it up on wikipedia.org: The actual date is 14. Juli 1789

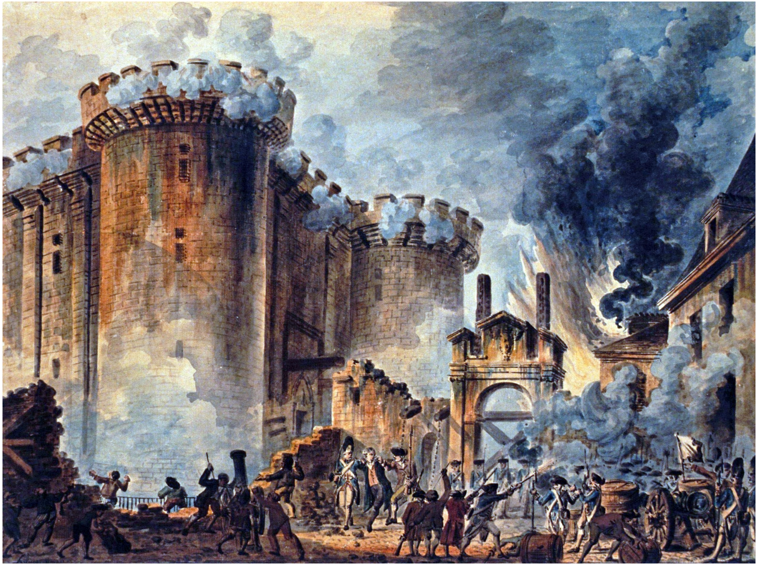


Figure: Prise de la Bastille by Jean-Pierre Louis Laurent Houel, 1789 (Image: Bibliothèque nationale de France)

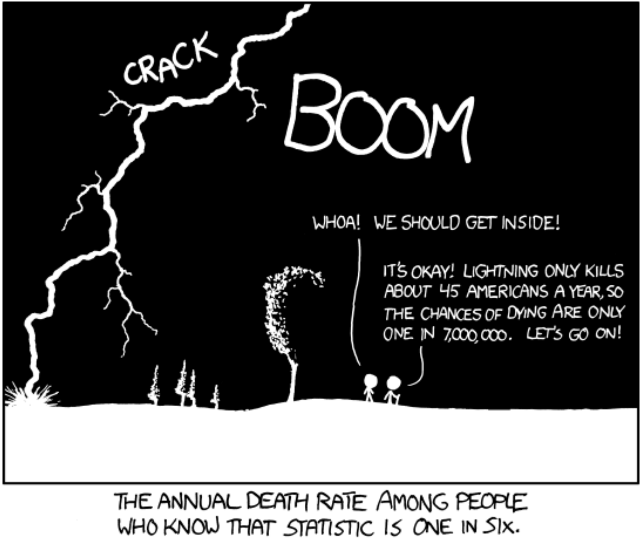


Figure: One more example concerning conditional probabilities (Image: xkcd)

Outline

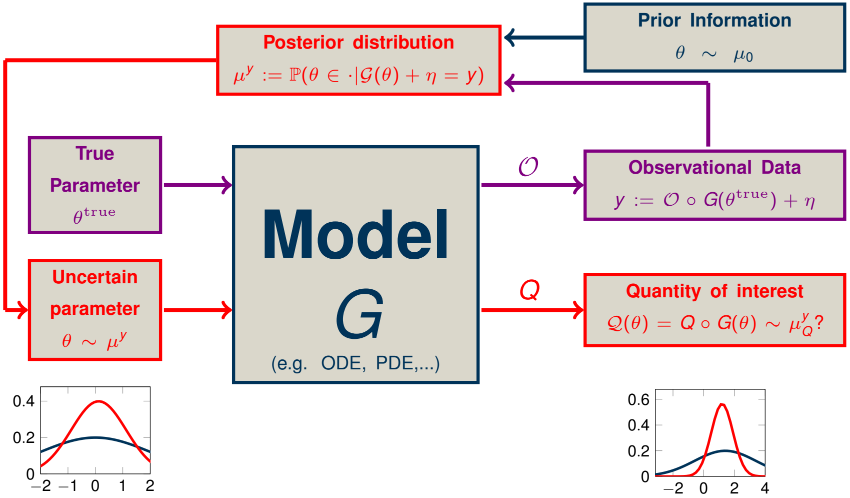
Bayesian Inverse Problem

Given data y and a prior distribution μ_0 - the parameter θ is a random variable: $\theta \sim \mu_0$.
Determine the posterior distribution μ^y, that is

$$\mu^y = \mathbb{P}(\theta \in \cdot | \mathcal{O} \circ G(\theta) + \eta = y)$$

The problem 'find μ^y' is well-posed

Bayesian Inverse Problem



Bayes' Theorem (revisited)

$$\underbrace{\mathrm{cpdf}(\theta | \mathcal{O} \circ G(\theta) + \eta = y)}_{\text{posterior}} = \underbrace{\mathrm{cpdf}(y|\theta)}_{\text{(data) likelihood}} \underbrace{\mathrm{mpdf}_1(\theta)}_{\text{prior}} / \underbrace{\mathrm{mpdf}_2(y)}_{\text{evidence}}$$

prior: Given by the probability measure μ_0

likelihood: $\mathcal{O} \circ G(\theta) - y = \eta \sim \mathrm{N}(0, \Gamma) \Leftrightarrow y \sim \mathrm{N}(\mathcal{O} \circ G(\theta), \Gamma)$

posterior: Given by the probability measure μ^y

evidence: Chosen as a normalising constant

How do we invert Bayesian?

Sampling based: Sample from the posterior measure μ^y

Importance Sampling
Markov Chain Monte Carlo
Sequential Monte Carlo/Particle Filters

Deterministic: Use a deterministic quadrature rule, to approximate μ^y

Sparse Grids
QMC

How do we invert Bayesian?

Sampling based: Sample from the posterior measure μ^y

Importance Sampling
Markov Chain Monte Carlo
Sequential Monte Carlo/Particle Filters

Deterministic: Use a deterministic quadrature rule, to approximate μ^y

Sparse Grids
QMC

Idea: Generate samples from μ^y.

Use these samples in a Monte Carlo manner to approximate the distribution of $\mathcal{Q}(\theta)$, where $\theta \sim \mu^y$.

Problem: We typically can't generate iid. samples of μ^y

- weighted samples of the wrong distribution (Importance Sampling, SMC)
- dependent samples of the right distribution (MCMC)

Idea: Generate samples from μ^y.

Use these samples in a Monte Carlo manner to approximate the distribution of $\mathcal{Q}(\theta)$, where $\theta \sim \mu^y$.

Problem: We typically can't generate iid. samples of μ^y

- weighted samples of the wrong distribution (Importance Sampling, SMC)
- dependent samples of the right distribution (MCMC)

Importance Sampling

Importance sampling applies directly Bayes' Theorem and uses the following identity:

$$\mathbb{E}_{\mu^y}[Q] = \mathbb{E}_{\mu_0}[Q \cdot \underbrace{\mathrm{cpdf}(y|\cdot)}_{\text{likelihood}}] / \underbrace{\mathbb{E}_{\mu_0}[\underbrace{\mathrm{cpdf}(y|\cdot)}_{\text{likelihood}}]}_{\text{evidence}}$$

Hence, we can integrate w.r.t. to μ^y, using only integrals w.r.t. μ_0.
In practice: Sample iid. from $(\theta_j : j = 1, ..., J) \sim \mu_0$ and approximate:

$$\mathbb{E}_{\mu^y}[Q] \approx J^{-1} \sum_{j=1}^{J} Q(\theta_j) \mathrm{cpdf}(y|\theta_j) / J^{-1} \sum_{j=1}^{J} \mathrm{cpdf}(y|\theta_j)$$

Markov Chain Monte Carlo

Construct an ergodic Markov chain $(\theta_n)_{n\geq 1}$ that is stationary with respect to μ^y.

- $\theta_n \sim \mu^y$ for n large,
- dependent samples can be used for MC type estimation
- some methods
  - Metropolis-Hastings MCMC
  - Gibbs sampling
  - Hamiltonian/Langevin MCMC
  - Slice sampling
  - ...
- often: accept-reject mechanisms

Deterministic Strategies

Several deterministic methods have been proposed

General issue: Estimating the model evidence is difficult
(this also contraindicates importance sampling)

Outline

Motivation: Forward and Inverse Problem

Conditional Probabilities and Bayes' Theorem

Bayesian Inverse Problem

Examples

Conclusions

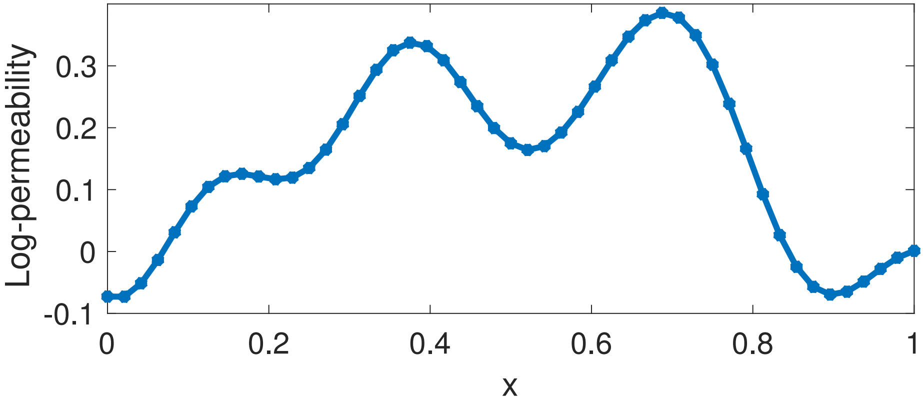
Example 1: 1D Groundwater flow with uncertain source

Consider the following partial differential equation on $D = [0, 1]$

$$-\nabla(k\nabla)p = f(\theta) \qquad \text{(on } D\text{)}$$
$$p = 0 \qquad \text{(on } \partial D\text{)},$$

where the diffusion coefficient k is known. The source term $f(\theta)$ contains one Gaussian-type source at position $\theta \in [0.1, 0.9]$.
(We solve the PDE using 48 linear Finite Elements.)

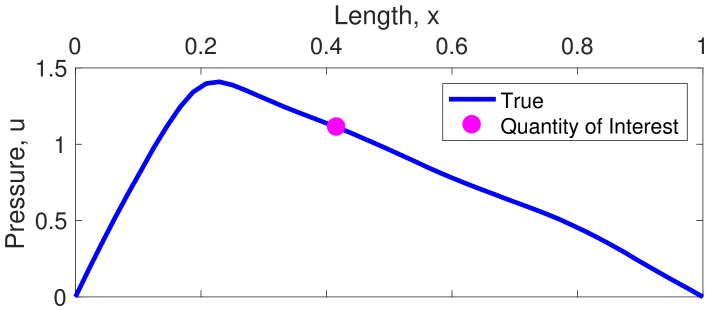
Example 1: (deterministic) log-Permeability



Example 1: Quantity of Interest

Considering the uncertainty in $f(\theta)$, determine the distribution of the Quantity of interest

$$\mathcal{Q} : [0.1, 0.9] \to \mathbb{R}, \theta \mapsto p(5/12).$$

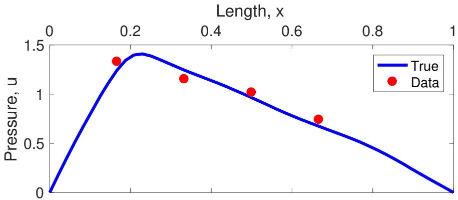


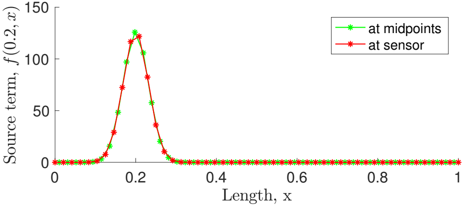
Example 1: Data

The observations are based on the observation operator $\mathcal{O}$, which maps

$$p \mapsto [p(2/12), p(4/12), p(6/12), p(8/12)],$$

given $\theta^{\text{true}} = 0.2$.





Example 1: Bayesian Setting

We assume uncorrelated Gaussian noise, with different variances:

(a) $\Gamma = 0.8^2$
(b) $\Gamma = 0.4^2$
(c) $\Gamma = 0.2^2$
(d) $\Gamma = 0.1^2$

Prior distribution $\theta \sim \mu_0 = \mathrm{Unif}[0.1, 0.9]$

Compare

- prior and different posteriors (with different noise levels)
- the uncertainty propagation of prior and the posteriors

(Estimations with standard Monte Carlo/Importance Sampling using $J = 10000$.)

Example 1: Bayesian Setting

We assume uncorrelated Gaussian noise, with different variances:

(a) $\Gamma = 0.8^2$
(b) $\Gamma = 0.4^2$
(c) $\Gamma = 0.2^2$
(d) $\Gamma = 0.1^2$

Prior distribution $\theta \sim \mu_0 = \mathrm{Unif}[0.1, 0.9]$

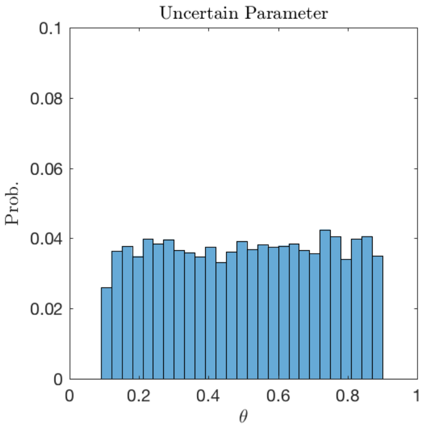
Compare

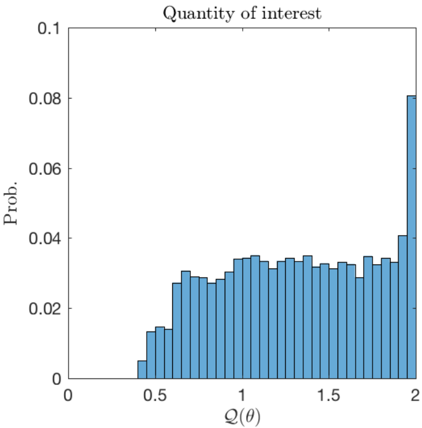
prior and different posteriors (with different noise levels)

the uncertainty propagation of prior and the posteriors

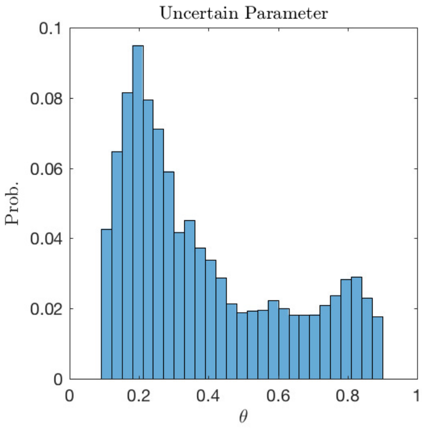
(Estimations with standard Monte Carlo/Importance Sampling using $J = 10000$.)

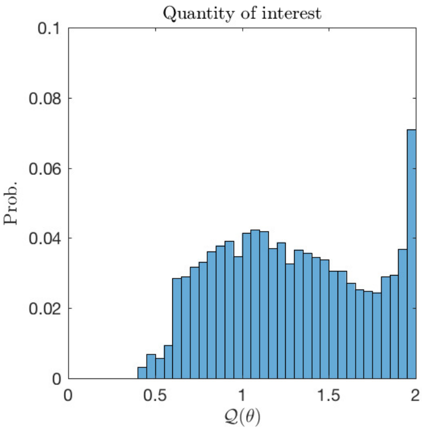
Example 1: No data (i.e. prior)



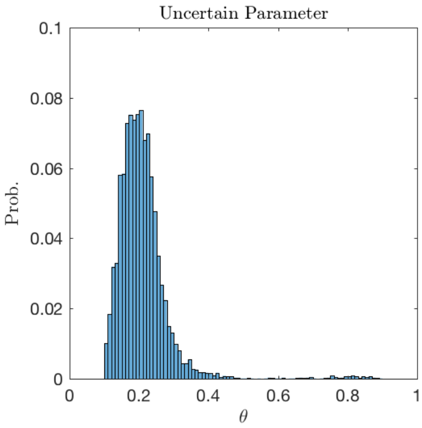


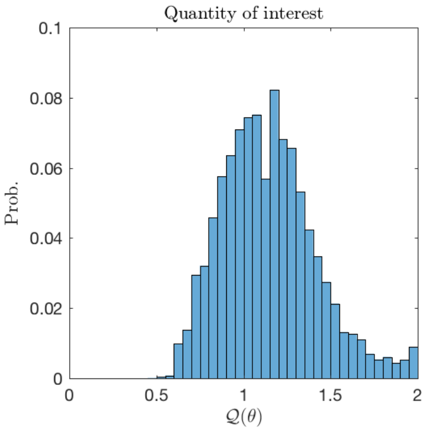
Example 1: Very high noise level $\Gamma = 0.8^2$



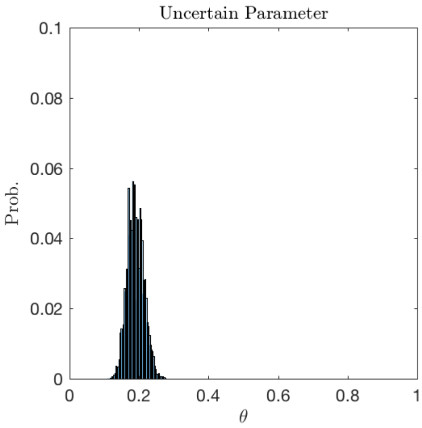


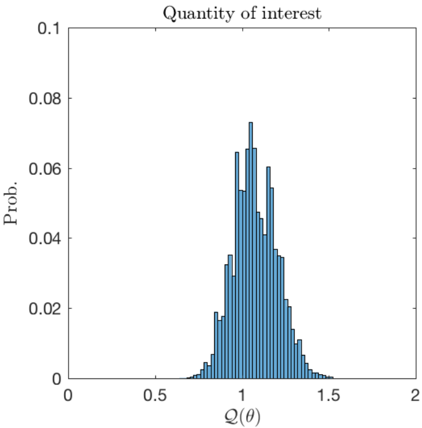
Example 1: High noise level $\Gamma = 0.4^2$



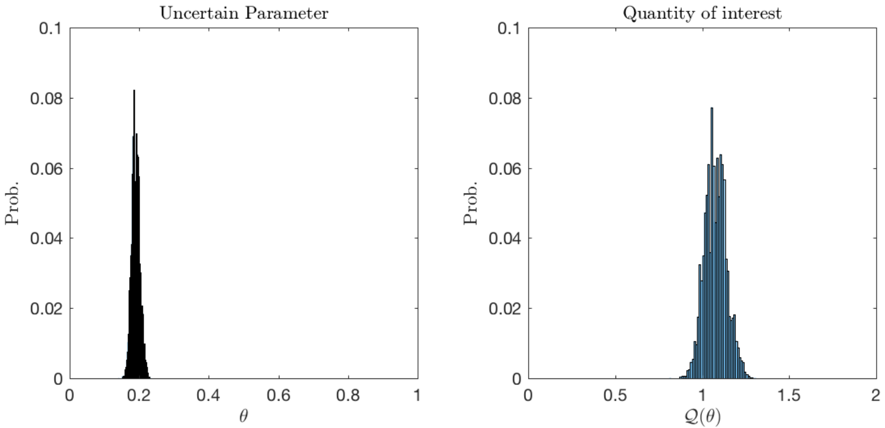


Example 1: Small noise level $\Gamma = 0.2^2$





Example 1: Very small noise level $\Gamma = 0.1^2$



Example 1: Summary

Smaller noise level $\Leftrightarrow$ less uncertainty in the parameter $\Leftrightarrow$ less uncertainty[2] in the quantity of interest

The unknown parameter can be estimated pretty well in this setting

Importance Sampling can be used in such simple settings.

[2]less uncertainty meaning ‘smaller variance’.

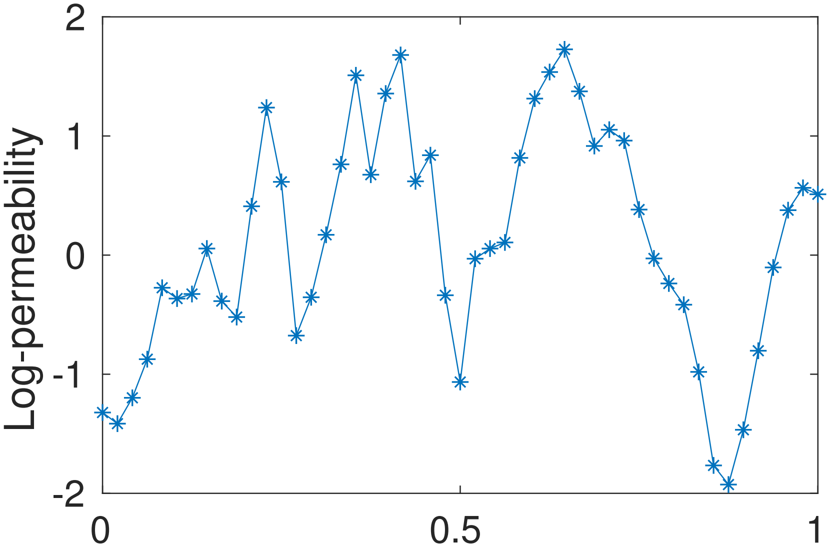
Consider again

$$
\begin{aligned}
-\nabla(k\nabla)p &= g(\theta) && \text{(on } D\text{)} \\
p &= 0 && \text{(on } \partial D\text{)},
\end{aligned}
$$

$\theta := (N, \xi_1, ..., \xi_N)$, where N is the number of Gaussian type sources and $\xi_1, ..., \xi_N$ are the positions of the sources (sorted ascendingly)

the log-permeability is known, but with a higher spatial variability

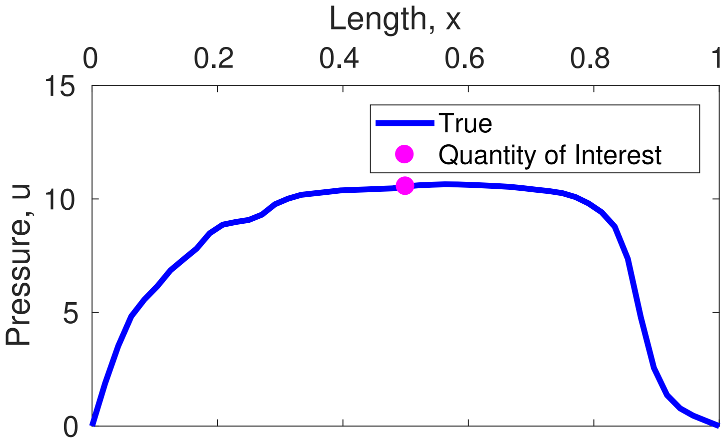
Example 2: (deterministic) log-Permeability



Example 2: Quantity of Interest

Considering the uncertainty in $g(\theta)$, determine the distribution of the Quantity of interest

$$\mathcal{Q} : [0.1, 0.9] \rightarrow \mathbb{R}, \theta \mapsto p(1/2).$$

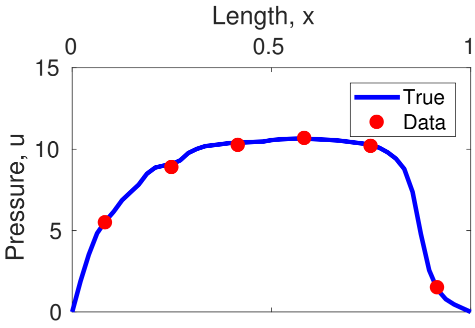


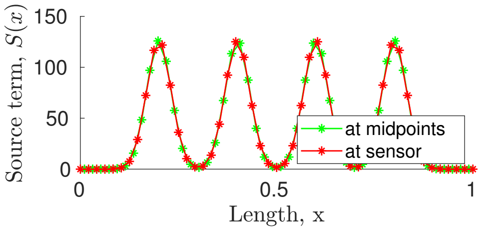
Example 2: Data

The observations are based on the observation operator $\mathcal{O}$, which maps

$$p \mapsto [p(1/12), p(3/12), p(5/12), p(7/12), p(9/12), p(11/12)],$$

given $\theta^{\text{true}} := (4, 0.2, 0.4, 0.6, 0.8)$.





Example 2: Bayesian Setting

We assume uncorrelated Gaussian noise with variance $\Gamma = 0.4^2$

Prior distribution $\theta \sim \mu_0$. μ_0 is given by the following sampling procedure:

1. Sample $N \sim \mathrm{Unif}\{1, ..., 8\}$
2. Sample $\xi \sim \mathrm{Unif}[0.1, 0.9]^N$
3. Set $\xi := \mathrm{sort}(\xi)$
4. Set $\theta := (N, \xi_1, ..., \xi_N)$

Compare prior and posterior and their uncertainty propagation (Estimations with standard Monte Carlo/Importance Sampling using $J = 10000$.)

Example 2: Bayesian Setting

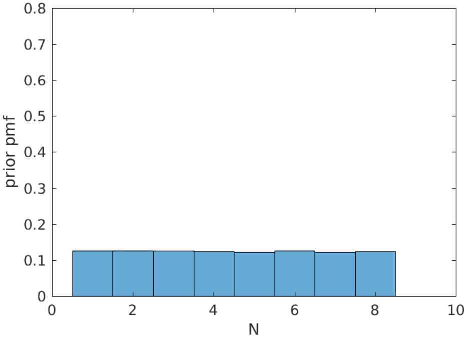
We assume uncorrelated Gaussian noise with variance $\Gamma = 0.4^2$

Prior distribution $\theta \sim \mu_0$. μ_0 is given by the following sampling procedure:

1. Sample $N \sim \mathrm{Unif}\{1, ..., 8\}$
2. Sample $\xi \sim \mathrm{Unif}[0.1, 0.9]^N$
3. Set $\xi := \mathrm{sort}(\xi)$
4. Set $\theta := (N, \xi_1, ..., \xi_N)$

Compare prior and posterior and their uncertainty propagation (Estimations with standard Monte Carlo/Importance Sampling using $J = 10000$.)

Example 2: Prior



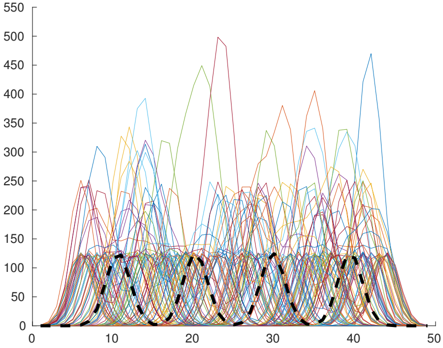


Figure: Prior distribution of N (left) and 100 samples of the prior distribution of the Source terms

Example 2: Posterior

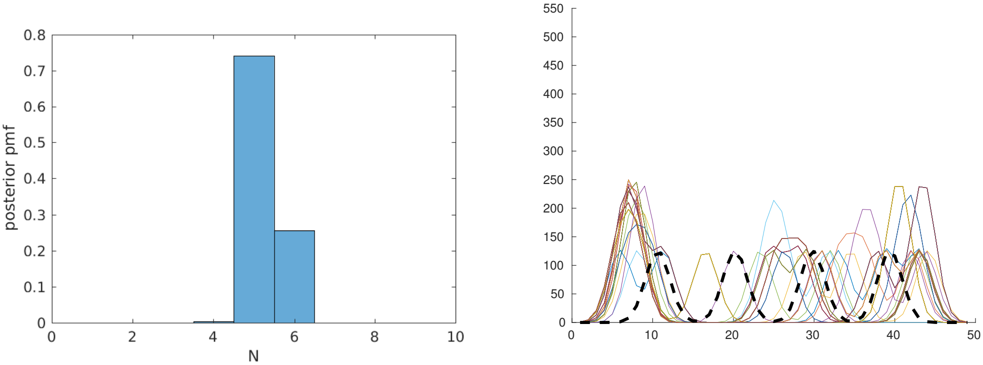


Figure: Posterior distribution of N (left) and 100 samples of the posterior distribution of the Source terms

Example 2: Quantity of Interest

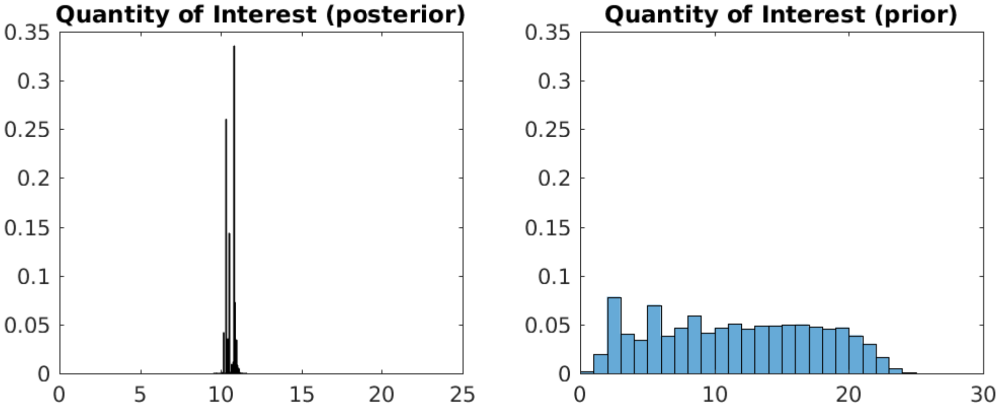


Figure: Quantities of interest, where the source term is distributed according to the prior (left) and posterior (right)

Example 2: Summary

Bayesian estimation is possible in ‘complicated settings’ (such as this transdimensional setting)

Importance Sampling is not very efficient

Outline

Messages to take home

+ Bayesian Statistics can be used to incorporate data into an uncertain model
+ Bayesian Inverse Problems are well-posed and thus a consistent approach to parameter estimation
+ Applying the Bayesian Framework is possible in many different settings, also in ones that are genuinely difficult (e.g. transdimensional parameter spaces)
- Solving Bayesian Inverse Problems is computationally very expensive
  - requires many forward solves
  - algorithmically complex

Messages to take home

+ Bayesian Statistics can be used to incorporate data into an uncertain model
+ Bayesian Inverse Problems are well-posed and thus a consistent approach to parameter estimation
+ Applying the Bayesian Framework is possible in many different settings, also in ones that are genuinely difficult (e.g. transdimensional parameter spaces)
- Solving Bayesian Inverse Problems is computationally very expensive
  - requires many forward solves
  - algorithmically complex

Messages to take home

- + Bayesian Statistics can be used to incorporate data into an uncertain model
- + Bayesian Inverse Problems are well-posed and thus a consistent approach to parameter estimation
- + Applying the Bayesian Framework is possible in many different settings, also in ones that are genuinely difficult (e.g. transdimensional parameter spaces)
- - Solving Bayesian Inverse Problems is computationally very expensive
  - requires many forward solves
  - algorithmically complex

Messages to take home

+ Bayesian Statistics can be used to incorporate data into an uncertain model
+ Bayesian Inverse Problems are well-posed and thus a consistent approach to parameter estimation
+ Applying the Bayesian Framework is possible in many different settings, also in ones that are genuinely difficult (e.g. transdimensional parameter spaces)
- Solving Bayesian Inverse Problems is computationally very expensive
  - requires many forward solves
  - algorithmically complex

How to learn Bayesian

- Various lectures at TUM:
  - Bayesian strategies for inverse problems, Prof. Koutsourelakis (Mechanical Engineering)
  - Various Machine Learning lectures in CS
- Speak with Prof. Dr. Elisabeth Ullmann or Jonas Latz (both M2)
- GitHub/latz-io
  - A short review on algorithms for Bayesian Inverse Problems
  - Sample Code (MATLAB)
  - These slides

How to learn Bayesian

Various Books/Papers

- Moritz Allmaras et al.- Estimating Parameters in Physical Models through Bayesian Inversion: A Complete Example (2013; SIAM Rev. 55(1))
- Jun Liu - Monte Carlo Strategies in Scientific Computing (2004; Springer)
- Sharon Bertsch McGrayne - The Theory that would not die (2011, Yale University Press)
- Christian Robert - The Bayesian Choice (2007, Springer)
- Andrew Stuart - Inverse Problems: A Bayesian Perspective (2010; in Acta Numerica 19)

Jonas Latz

`Input/Output: www.latz.io`