Introduction to Uncertainty Quantification for Bayesian Inverse Problems

Babak Maboudi - day 1 - Jyväskylä summer school 2025

What are inverse problems?

- When we want to understand hidden causes from indirect measurements.
- It is best understood by examples!

Examples of Inverse Problems

X-ray Computed Tomography (CT) or CAT scan

Anna Bertha Ludwig's hand

X-ray by Wilhelm Röntgen

1895

First X-ray image in space

2025

Examples of Inverse Problems

X-ray Computed Tomography (CT) or CAT scan

X-ray radiography

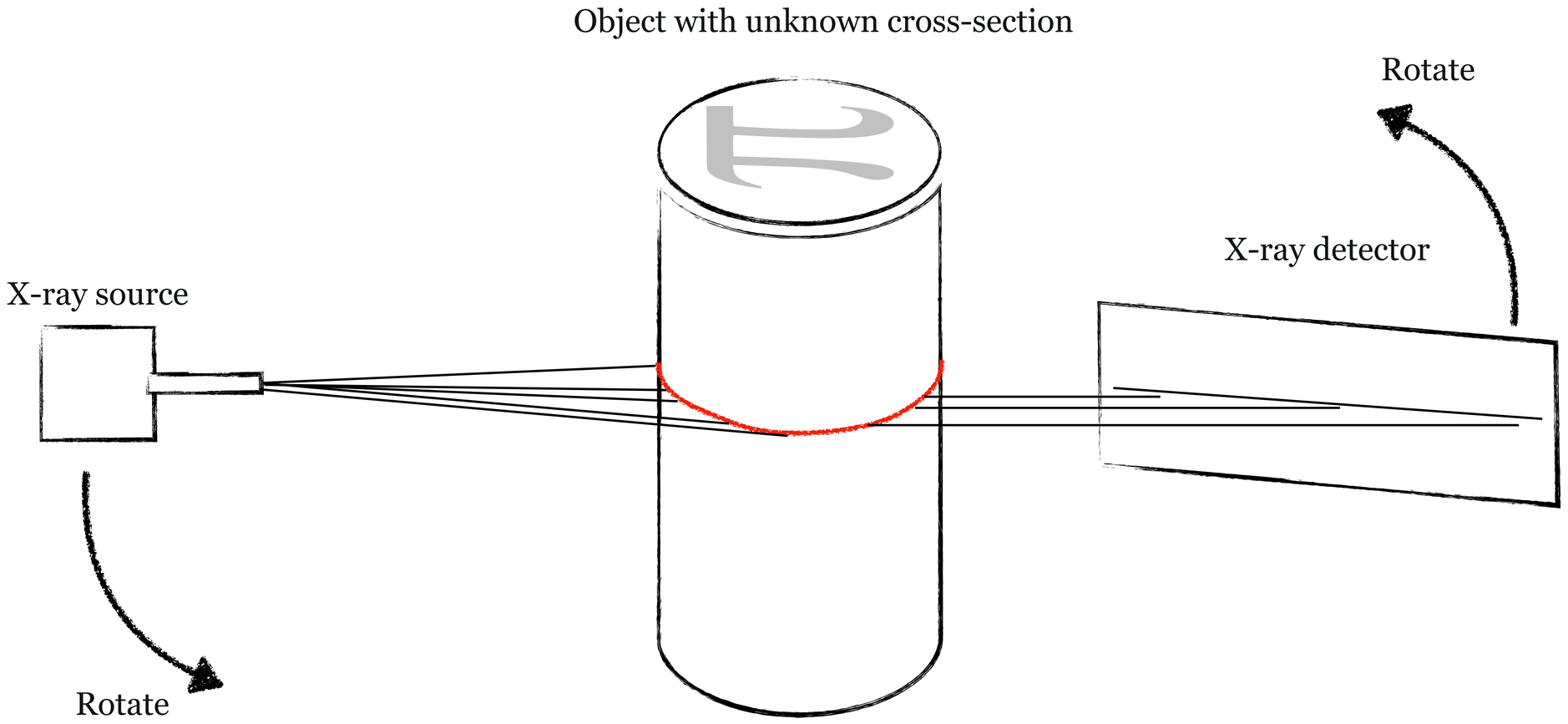
One X-ray image

X-ray computed tomography (CT)

Sequence of X-ray images

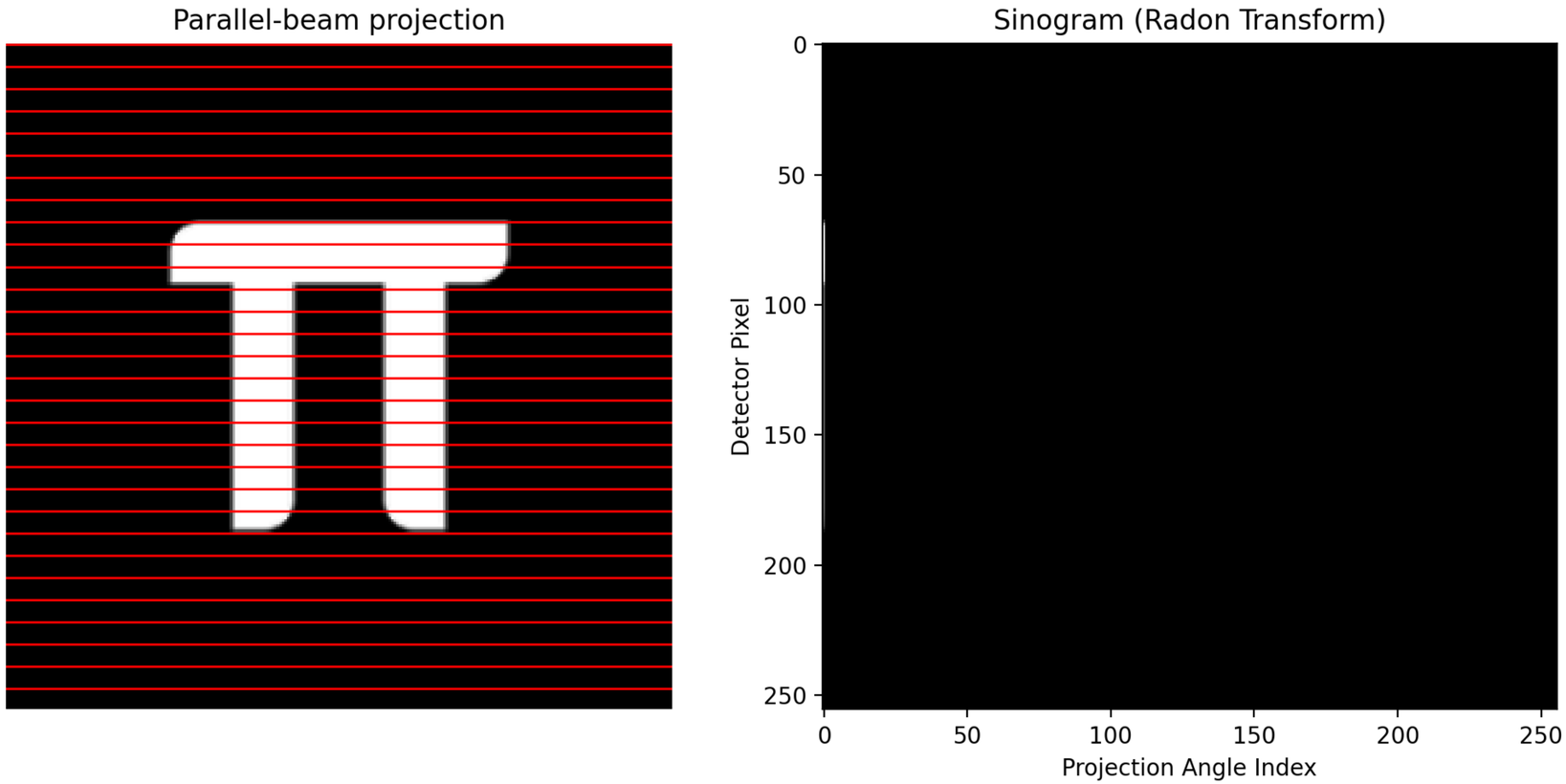
Examples of Inverse Problems

X-ray CT, a 2D example



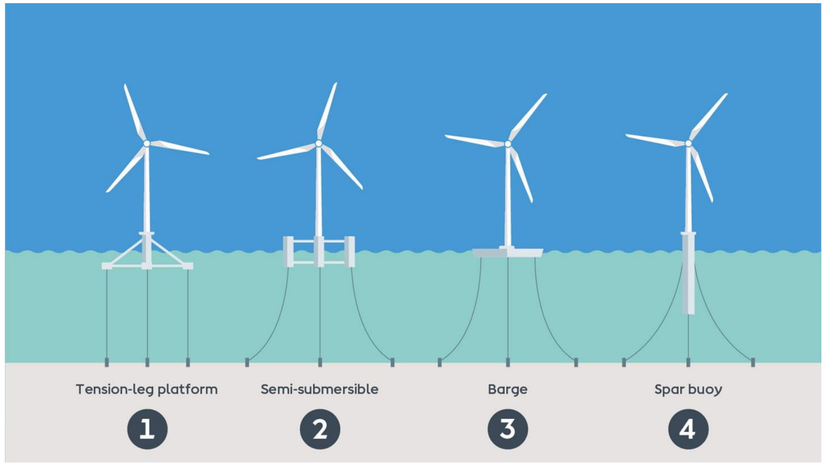
Examples of Inverse Problems

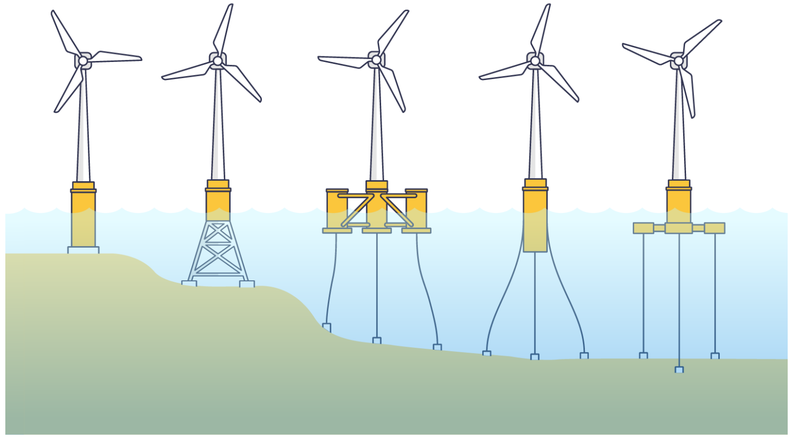
X-ray CT, a 2D example



Examples of Inverse Problems

Ocean Floor Detection/Exploration





Examples of Inverse Problems

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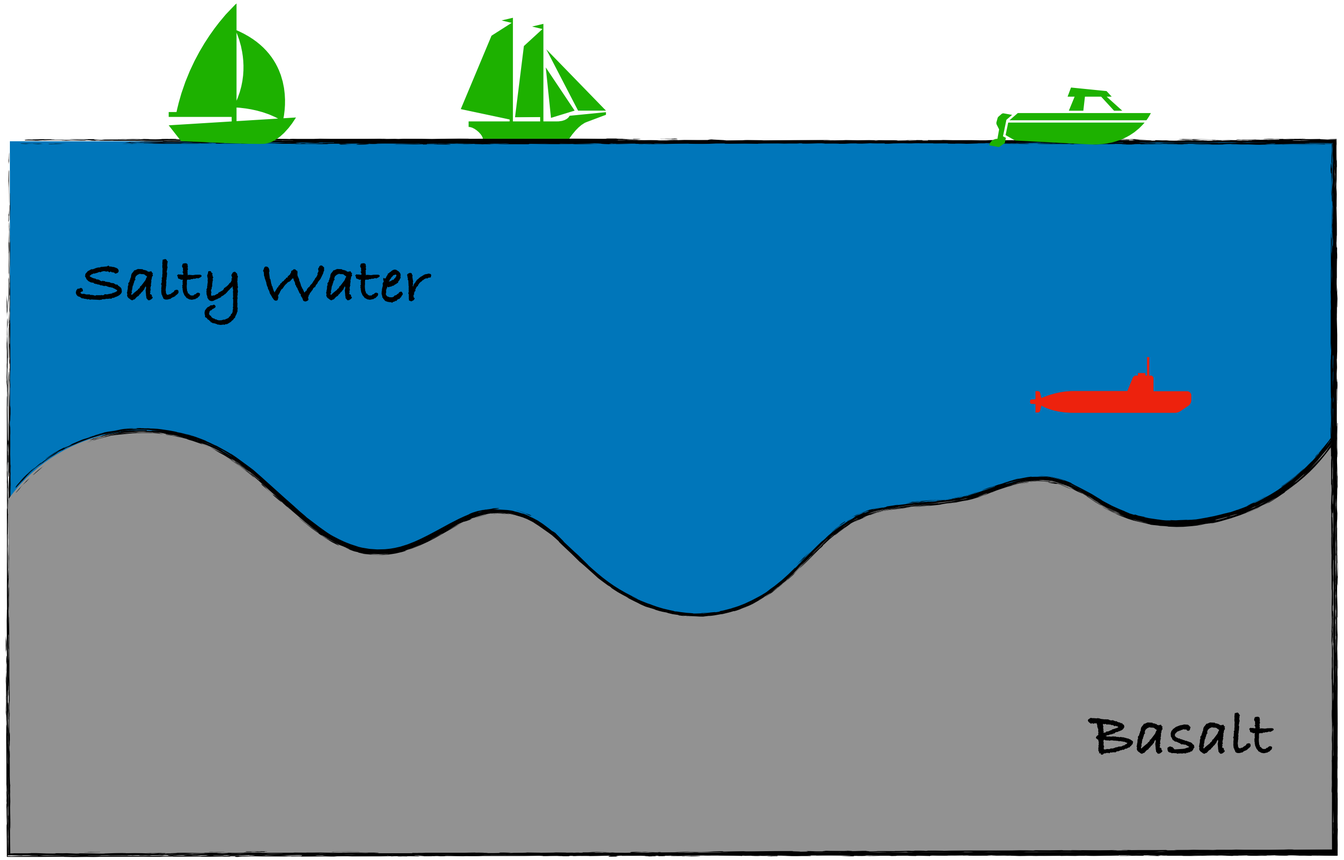
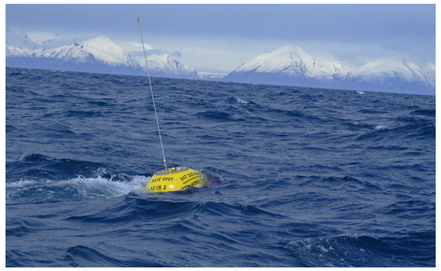
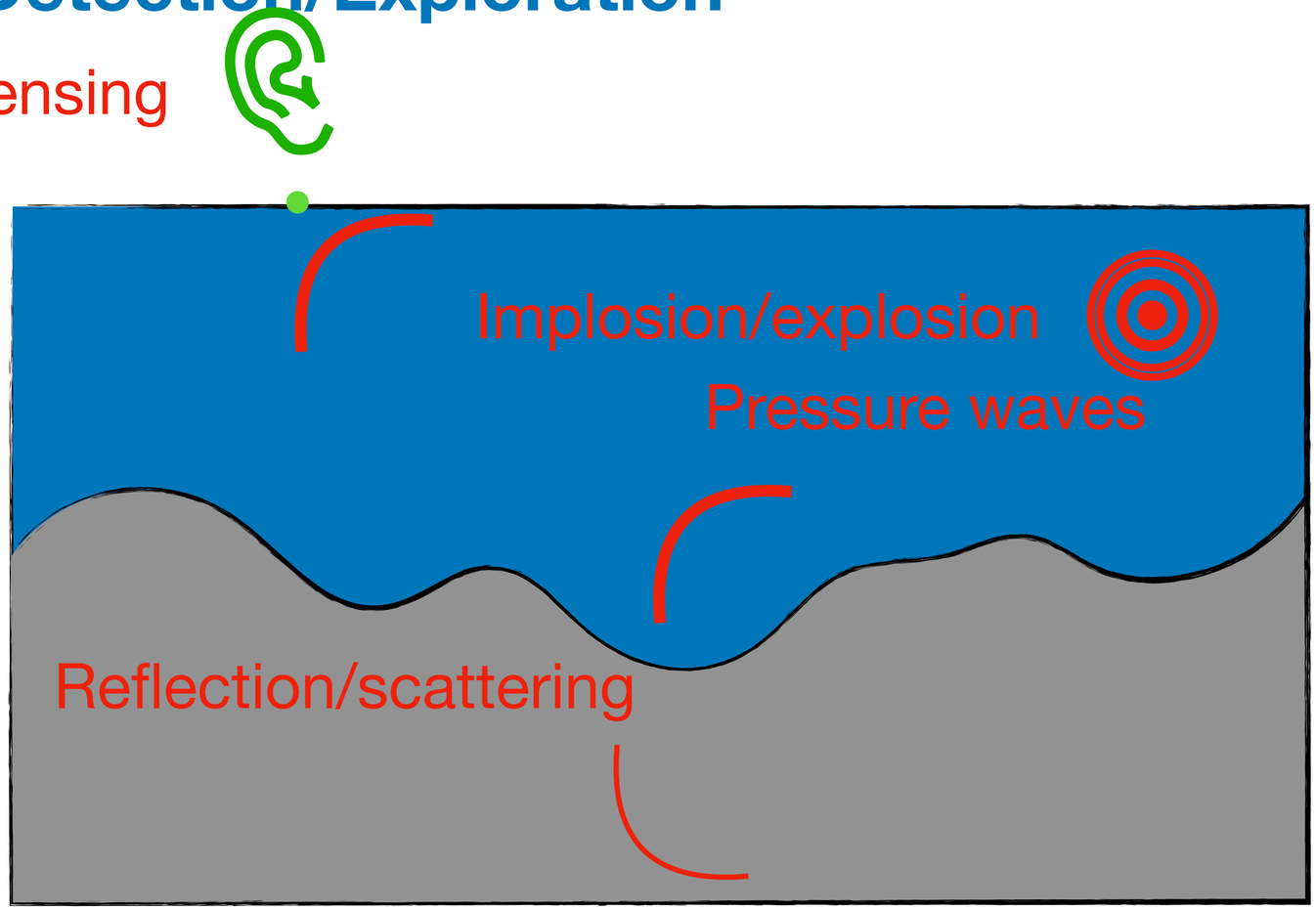


Examples of Inverse Problems

Ocean Floor Detection/Exploration

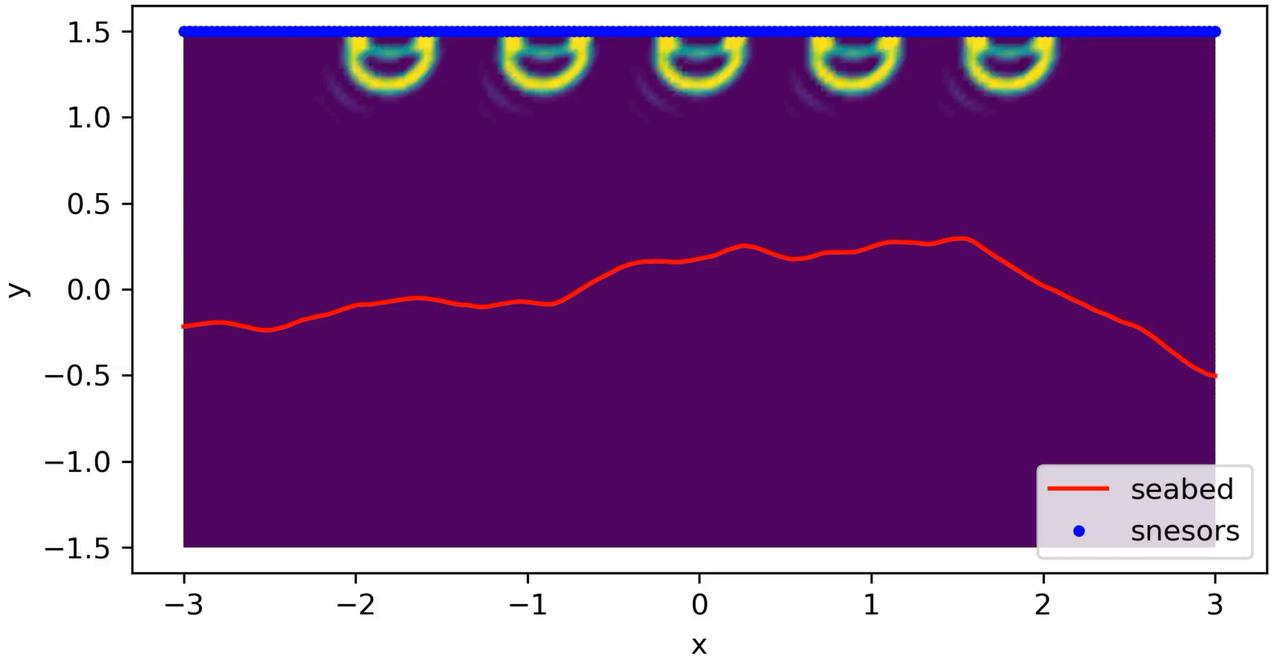


Wave Buoys



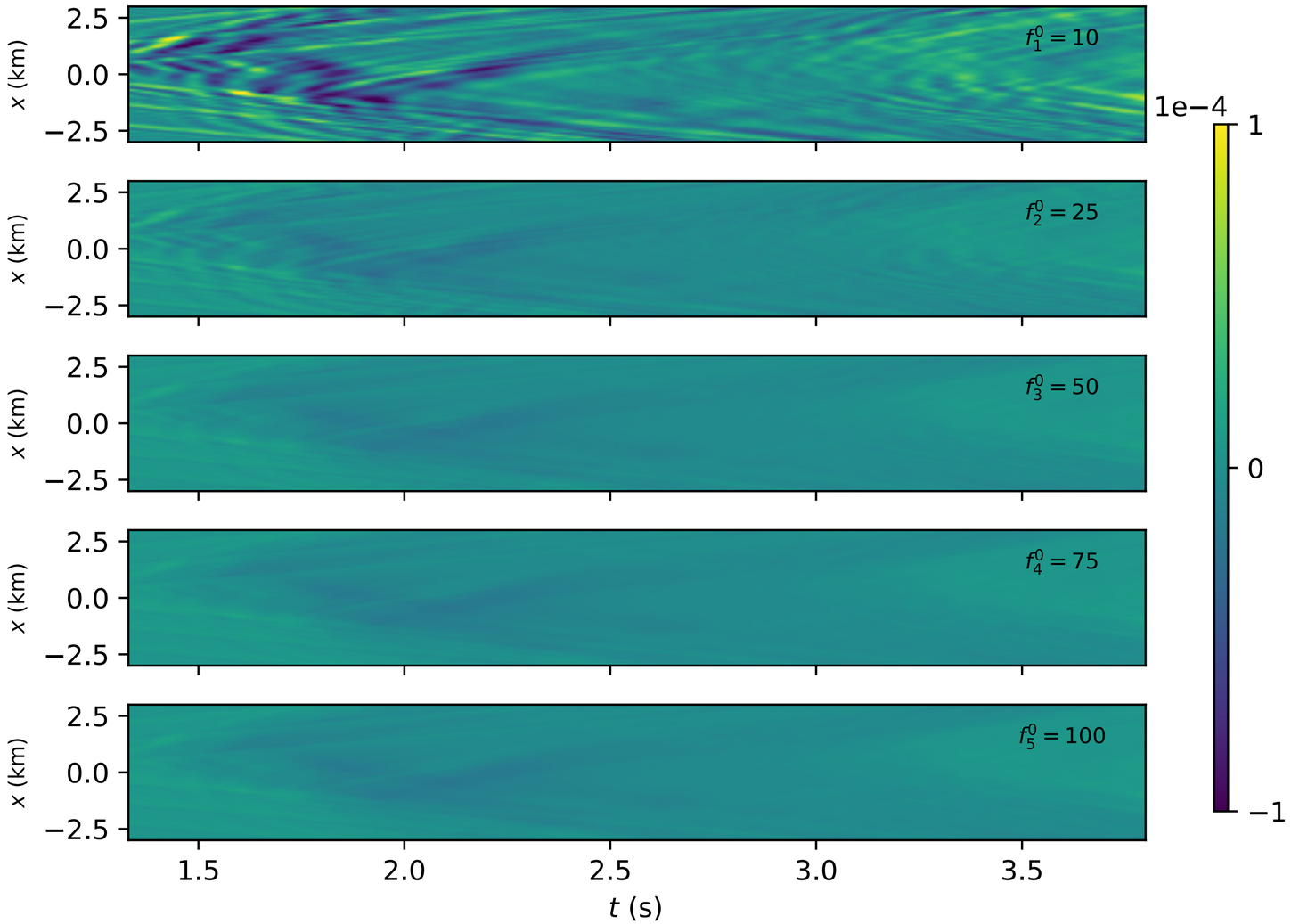
Examples of Inverse Problems

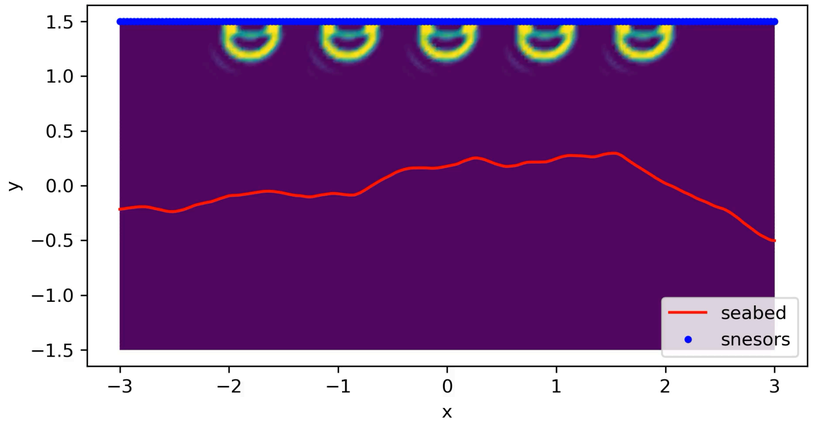
Ocean Floor Detection/Exploration

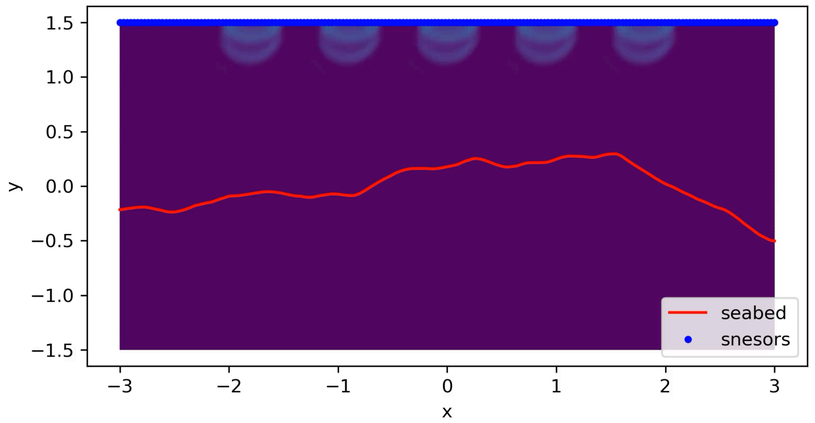


Examples of Inverse Problems

Ocean Floor Detection/Exploration

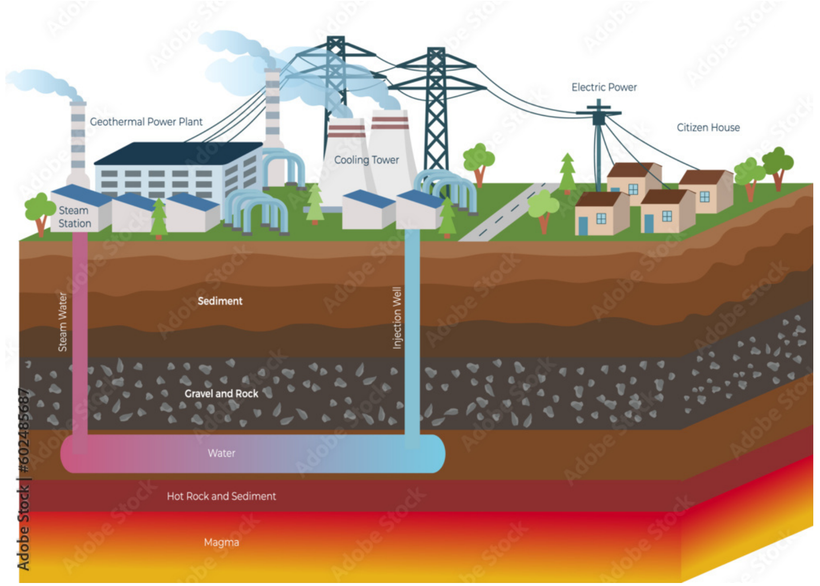






Examples of Inverse Problems

Geo-thermal Power stations (Motivation for Course Project)



Examples of Inverse Problems

- A typical formulation of an inverse problem

$$\mathbf{y} = F(\mathbf{x}) + \varepsilon$$

  - Here $\mathbf{x}$ is a mathematical representation of the unknown. It can be a parameter in $\mathbb{R}^+$, a vector of parameters in $\mathbb{R}^d$, a function in a function space, …
  - F is called the forward operator and is the (physical or approximate) process that creates noise-free measurements from a known $\mathbf{x}$.
  - ε is the noise in the measurement instruments.
  - $\mathbf{y}$ is the raw measurement.

- Discuss in groups what are $\mathbf{x}$, $\mathbf{y}$, ε and F in the examples we discussed previously.

Uncertainty in Inverse Problems

Exercise 1

- In each of these examples investigate what are sources of uncertainty?
  - X-ray CT
  - Ocean floor detection with waves
  - Geo-thermal power station (both for exploration and monitoring)
- What are the consequences of uncertainties in each case?

Uncertainty in Inverse Problems

Exercise 2

- Choose an inverse problem of your choice. Investigate what are the sources of uncertainties.
- What are the consequences of uncertainty in your example?

Teaching Objectives of This Course

By the end of this course:

- You can formulate an inverse problem in a statistical setting.
- You can incorporate prior knowledge into the statistical problem in terms of a prior distribution.
- You can use the Bayes' theorem to formulate the solution to an inverse problem as the posterior distribution.
- You can write an algorithm and a Python code that can explore the posterior distribution with a sampling method.
- You can interpret samples of the posterior distribution as level of uncertainty (quantified uncertainty).
- You can perform uncertainty quantification for both linear and non-linear inverse problems.
- You will deliver outputs through teamwork.

What to expect in this course?

- You must work in groups of 3.
- You need to write codes in Python. You need numpy, matplotlib and scipy.
- We will have an active learning teaching method (appose to in-active students).
- Every session will have “homework” which we will do during the lectures.
- Ideally all homework will be finished in class.
- You will hand-in selected homework as your course report in groups of 3. You will be evaluated based on the final report.
- Advice: Start your Latex report as we go through the week.

Course Overview

- Day 1: Introduction to Inverse Problems, Uncertainty Quantification and revision on basic probability theory.
- Day 2: Markov chain and acceptance/rejection sampling.
- Day 3: The famous random-walk Metroplis-Hastings algorithm.
- Day 4: Choices of priors for Bayesian inverse problems.
- Day 5: Continuous and differentiable priors for Bayesian inverse problems.

Bayesian vs. Frequentist Debate

Source for the coin analogy:

Cassie Kozyrkov

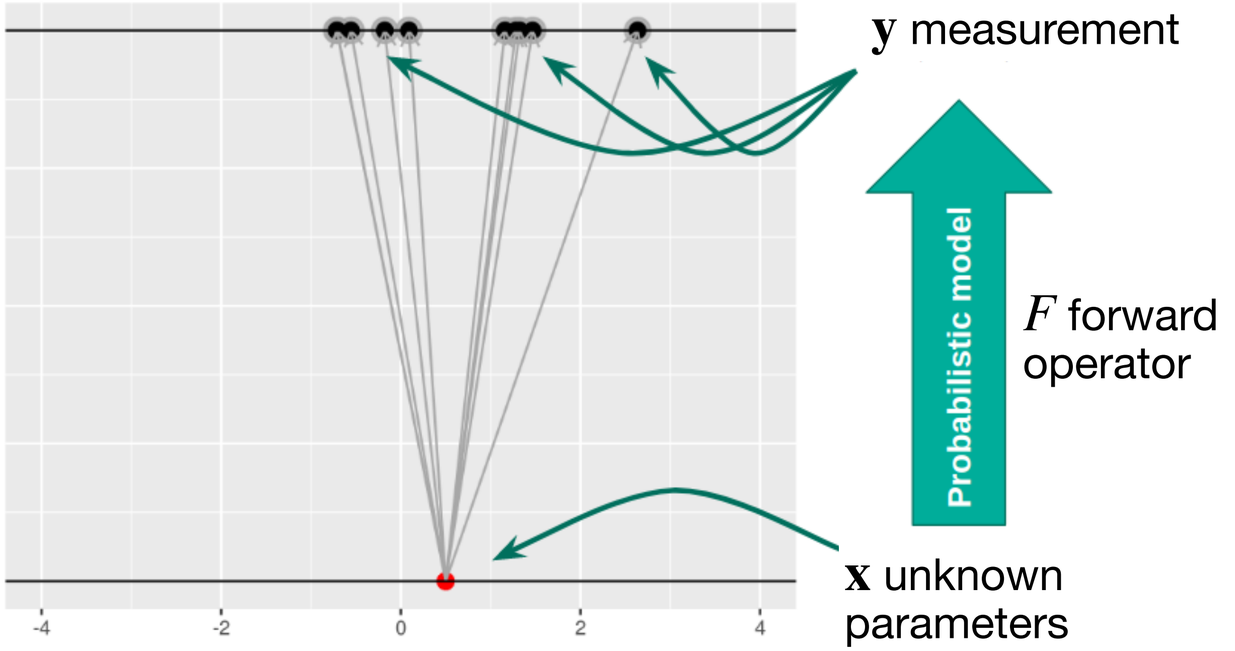
Are you Bayesian or Frequentist?

https://www.youtube.com/watch?v=GEFxFVESQXc&t=2s

Inverse Problems

A generic view

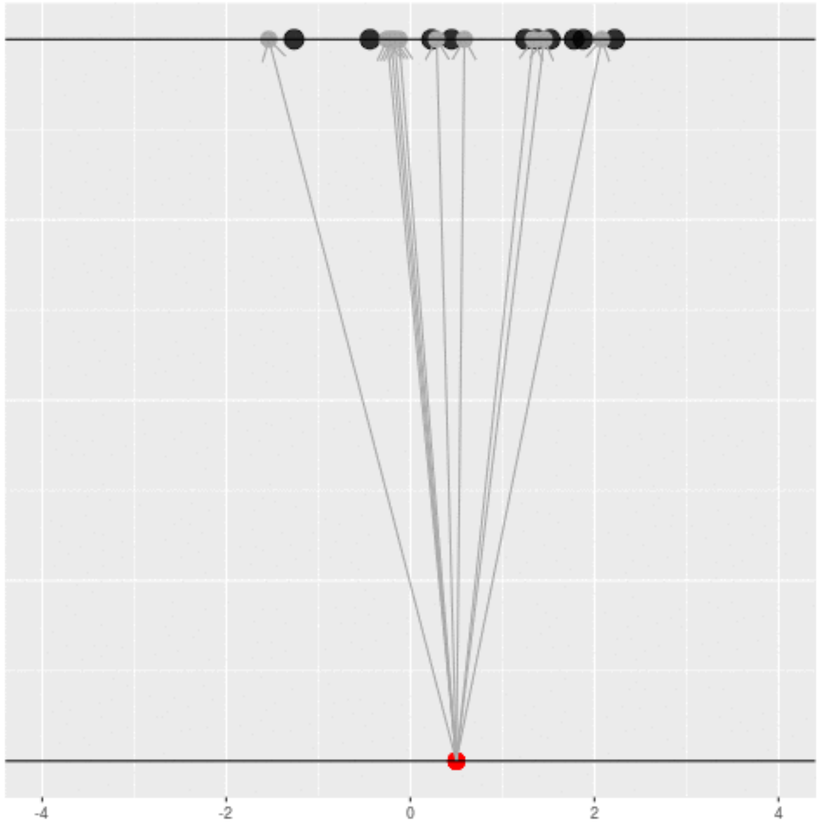
- Recall
  - $\mathbf{x}$ is the unknown
  - $\mathbf{y}$ is the measurement
  - F is the forward operator



Inverse Problems

A frequentist approach

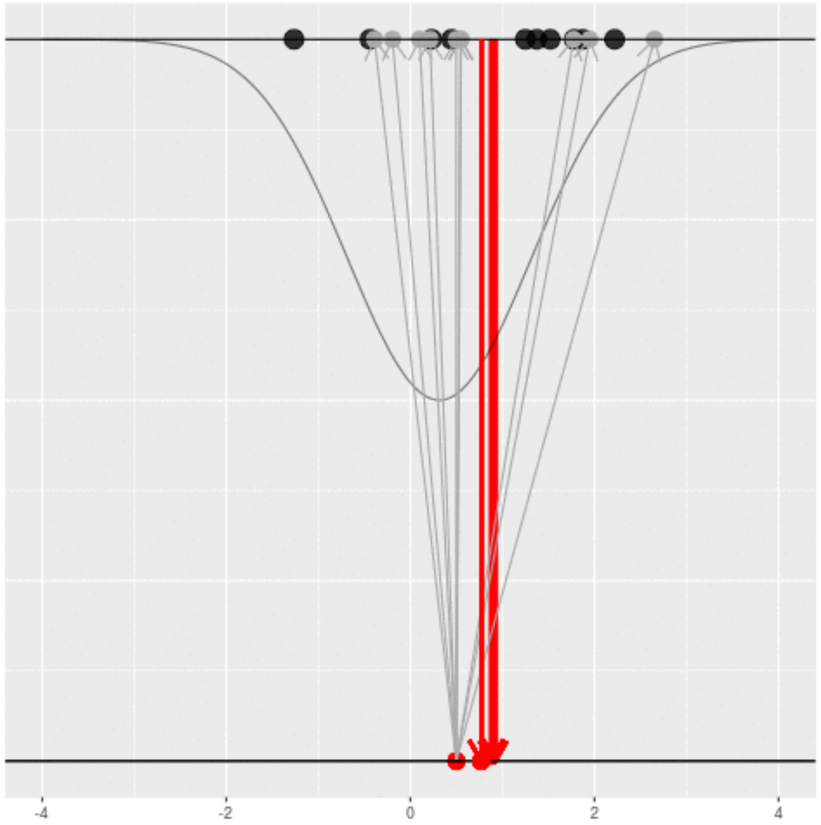
- There is a true parameter $\mathbf{x}$
- Due to noise, every measurement is different, i.e., same parameter can result in different measurement data.



Inverse Problems

A frequentist uncertainty quantification

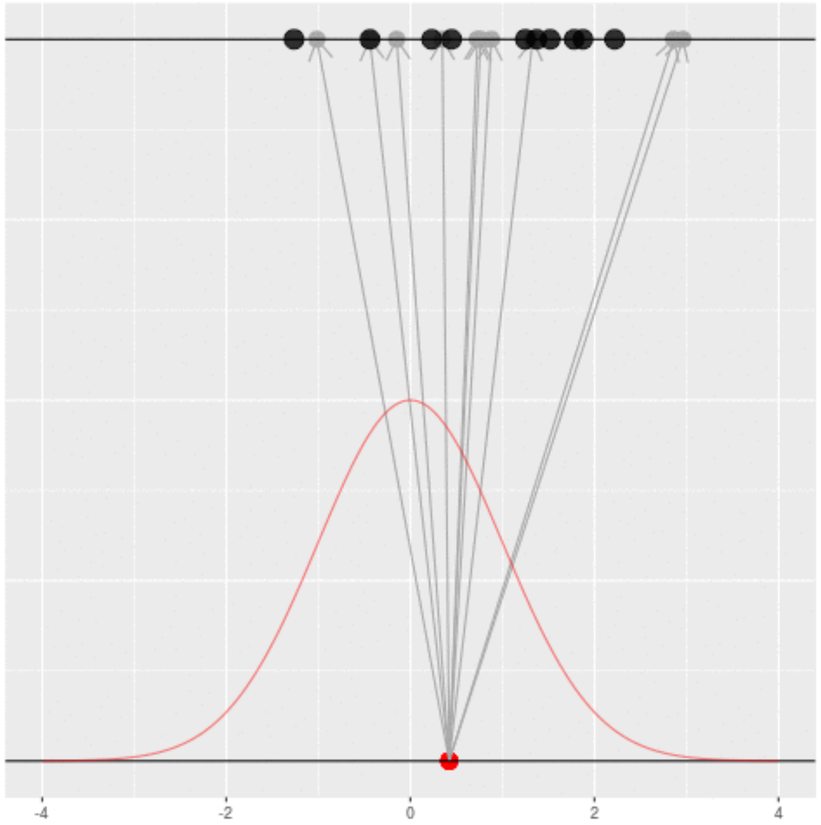
- Pick an estimate strategy.
- The range these estimates create, if we repeated the experiment, quantifies the uncertainty.



Inverse Problems

A Bayesian approach

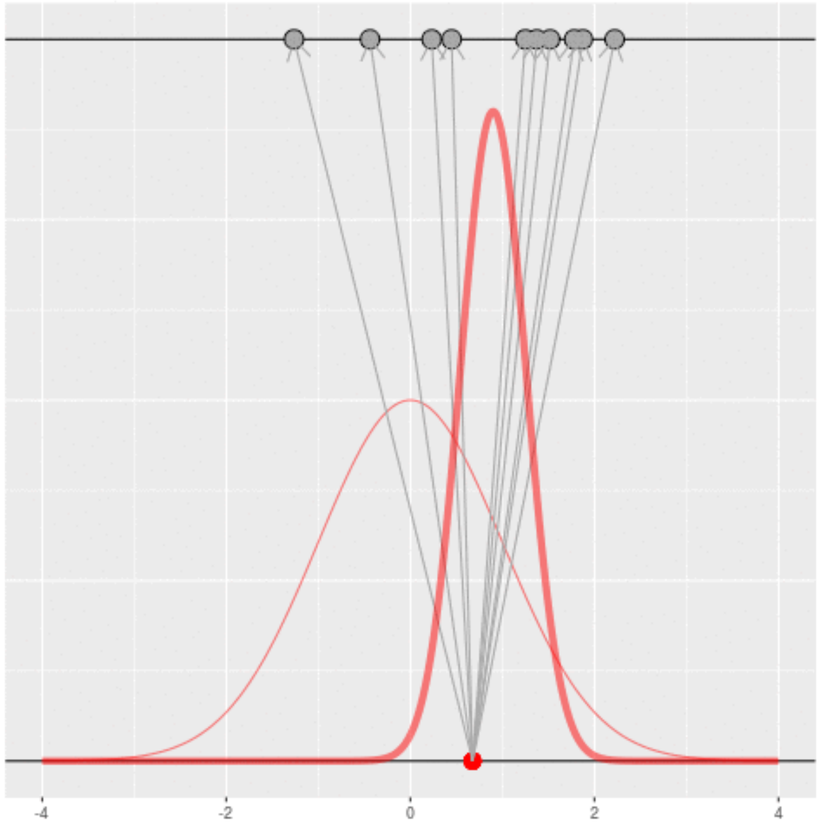
- There is a no true parameter **x**
- We have an opinion, or a prior belief on what the value of **x** is.
- Different parameters can create different measurement data.



Inverse Problems

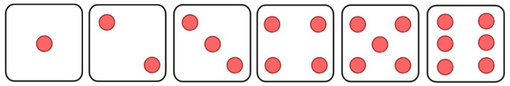
A Bayesian uncertainty quantification

- We delete the parameters that does not match with data.
- What remains is called the posterior.
- The uncertainty is then interpreted as the shape of the posterior.



Recap

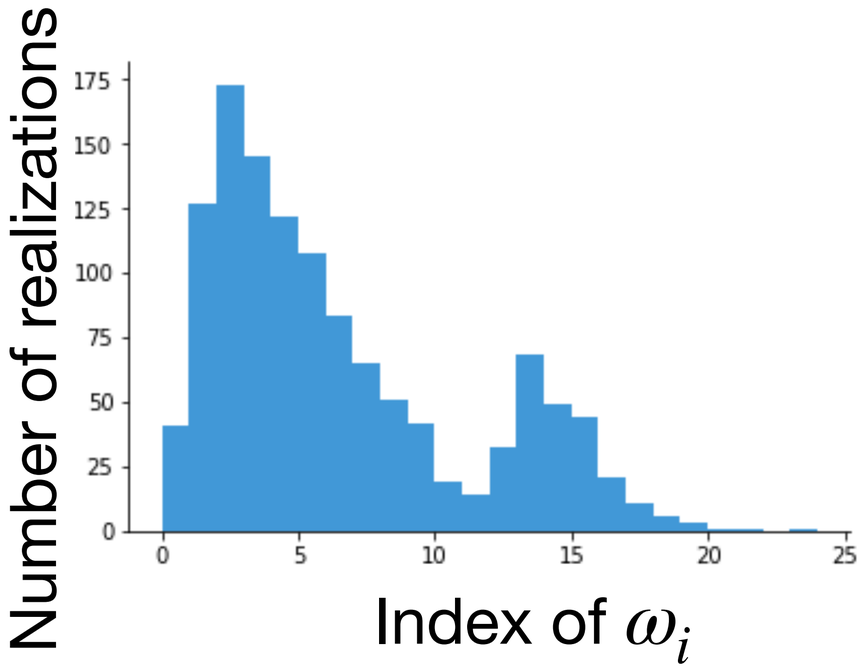
Random variables

- We model random events that takes values in a set Ω as Ω-valued random variables and write them with capital letters, e.g., $X, Y, \ldots$
  - Let $A = \{$  $\}$, then a dice roll is an A-valued random variable.
  - Let $B = \{$  $\}$, then a flip of a (Finnish) 1 Euro coin is a B-valued random variables.
  - Let $C = [0,3]$ meters, then measuring hight of people is a C-valued random variable.
  - Let D be the set of continuous and finite paths in 3D space. Then the path of a mosquito in the air is a D-valued random variable.

Recap

Histogram

- Let X be an Ω-valued random variables. Then under repeated realizations of X we record the outcomes in a sequence $\omega_1, \omega_2, \omega_1, \omega_4 \ldots$ A histogram is then a frequency plot.



Recap

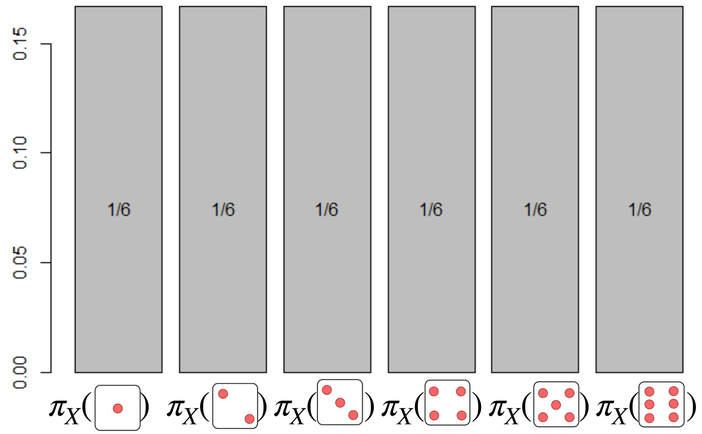
Density function

- The law, under which, a random variable behaves is called a distribution of a random variable.
  - For X being a fair dice roll, the distribution assigns equal probability of seeing each number.
- We can (sometimes) express a distribution using a density function. Which contains the “probability” of each event.
  - We represent a density as $\pi_X(\mathbf{x})$: This means the probability of the Ω -valued random variable X for the outcome $\mathbf{x} \in \Omega$.

Recap

Examples of Density function

- Let X be a random variable of a fair dice roll. Then we can represent its density function as



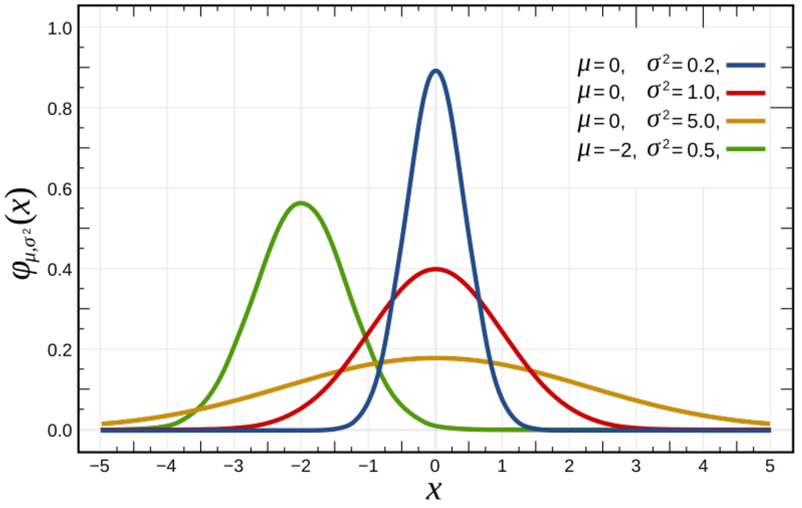
Recap

Examples of Density function

- Let X be an $\mathbb{R}$-valued random variable. Then the wrong way to think about its density function is to think of a function that assigns probability to each point $\mathbf{x} \in \mathbb{R}$. Although this analogy is wrong, we can use it for the purpose of this course.

- Normal distribution is a classic example. In this case:

$$\pi_X(\mathbf{x}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\mathbf{x}-\mu)^2}{2\sigma^2}\right)$$



Recap

Examples of Density function - multivariate Gaussian

- Let X be an $\mathbb{R}^n$-valued Gaussian random variable. Then there is a vector $\mathbf{m} \in \mathbb{R}^n$ (the mean) and a symmetric and positive-definite matrix $\mathscr{C}$ (the covariance matrix) such that the density function of X is

$$\pi_X(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n \, |\mathscr{C}|}} \exp(-\frac{1}{2}(\mathbf{x}-\mathbf{m})^T \mathscr{C}^{-1}(\mathbf{x}-\mathbf{m}))$$

  and we write $X \sim \mathcal{N}(\mathbf{m}, \mathscr{C})$.

- In this course we only consider zero-mean random variables.

Recap

Exercise

- What is the difference between a density function of random variable X and a histogram of a random variable X?

Statistical Formulation of Inverse Problems

- Recall formulation of an inverse problem.

$$\mathbf{y} = F(\mathbf{x}) + \varepsilon$$

- We define random variables to replace the components of the inverse problem.
  - define X to be the random variable of the unknown $\mathbf{x}$.
  - Define Y to be the random variable of the measurement $\mathbf{y}$.
  - Similarly E is the random variable of ε.
  - Note that randomness in F comes from $\mathbf{x}$, and F itself is not necessarily random.

Statistical Formulation of Inverse Problems

- The statistical modeling of the inverse problem is:

$$Y = F(X) + E$$

- What we need to define now is $\pi_X(\mathbf{x}), \pi_E(\mathbf{e})$:
  - $\pi_X(\mathbf{x})$ is called the prior density. It shows our belief (the probability) of any value $\mathbf{x}$ the.
  - $\pi_E(\mathbf{e})$ is the distribution of noise. Every sensor comes with a description of how precise measurements are.
- The solution to the inverse problem is then the conditional random variable $X \mid Y$, a.k.a. *the posterior*. We can also describe the posterior in terms of its density function.

$$\pi_{X|Y=\mathbf{y}}(\mathbf{x})$$

Statistical Formulation of Inverse Problems

Bayes' rule

- We now use the Bayes' rule to simplify the posterior density function:

$$\pi_{X|Y=\mathbf{y}}(\mathbf{x}) = \frac{\pi_{Y|X=\mathbf{x}}(\mathbf{y})\pi_X(\mathbf{x})}{\pi_Y(\mathbf{y})}$$

  - $\mathbf{y}$ is measurement data and we have it!
  - $\pi_{X|Y=\mathbf{y}}(\mathbf{x})$ is the posterior density function. This is what we want to compute.
  - $\pi_X(\mathbf{x})$ is the prior density function. This is something that we have.
  - $\pi_{Y|X}(\mathbf{y})$ is called the likelihood density function and is easy to evaluate (next slide).
  - $\pi_Y(\mathbf{y})$ is the probability of data. This is very hard to evaluate but generally unimportant. We find a way to deal with this term in the next days.

Statistical Formulation of Inverse Problems

Likelihood distribution $\pi_{Y|X}(\mathbf{y})$

- Recall a statistical inverse problem
$$Y = F(X) + E$$
- We want to compute $\pi_{Y|X=\mathbf{x}}(\mathbf{y})$. This means that we have $\mathbf{x}$:
$$Y = F(\mathbf{x}) + E$$
- Suppose that E is a Gaussian, i.e., $E \sim \mathcal{N}(0,\sigma^2)$, or $\pi_E(\mathbf{e}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\mathbf{e}^2/(2\sigma^2))$.
- $F(\mathbf{x})$ is not random! Take it to the other side of the equation and write:
$$Y - F(\mathbf{x}) = E$$
- Can you guess what is the density function of the left-hand-side? $F(\mathbf{x})$ can be a mean of a distribution.

Statistical Inversion

Linear problem with Gaussian noise

- Recall a statistical inverse problem

$$Y = F(X) + E,$$

  Let

  - $X \sim \mathcal{N}(0,1)$, with

$$\pi_X(\mathbf{x}) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\mathbf{x}^2}{2}\right)$$

  - $E \sim \mathcal{N}(0,\sigma^2)$, with

$$\pi_E(\varepsilon) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\varepsilon^2}{2\sigma^2}\right)$$

  - $\pi_{Y|X=\mathbf{x}} \sim \mathcal{N}(F(\mathbf{x}), \sigma^2)$, with

$$\pi_{Y|X=\mathbf{x}}(\mathbf{y}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\mathbf{y} - F(\mathbf{x}))^2}{2\sigma^2}\right)$$

  - Since $\mathbf{y}$ is already measured, then $\pi_Y(\mathbf{y})$ is a constant.

Statistical Inversion

Linear problem with Gaussian noise

- Now we can put everything into the Bayes' rule:

$$\pi_{X|Y=\mathbf{y}}(\mathbf{x}) = \frac{\pi_{Y|X=\mathbf{x}}(\mathbf{y})\pi_X(\mathbf{x})}{\pi_Y(\mathbf{y})}$$

- This gives us the relation:

$$\pi_{X|Y=\mathbf{y}}(\mathbf{x}) = \frac{1}{c}\exp\left(-\frac{(\mathbf{y}-F(\mathbf{x}))^2}{2\sigma^2}\right)\exp\left(-\frac{\mathbf{x}^2}{2}\right)$$

- The constant c is referred to as the normalization constant.

Statistical Inversion

Linear problem with Gaussian noise - multivariate case $\mathbf{x} \in \mathbb{R}^n$

- Now we can put everything into the Bayes' rule:

$$\pi_{X|Y=\mathbf{y}}(\mathbf{x}) = \frac{\pi_{Y|X=\mathbf{x}}(\mathbf{y})\pi_X(\mathbf{x})}{\pi_Y(\mathbf{y})}$$

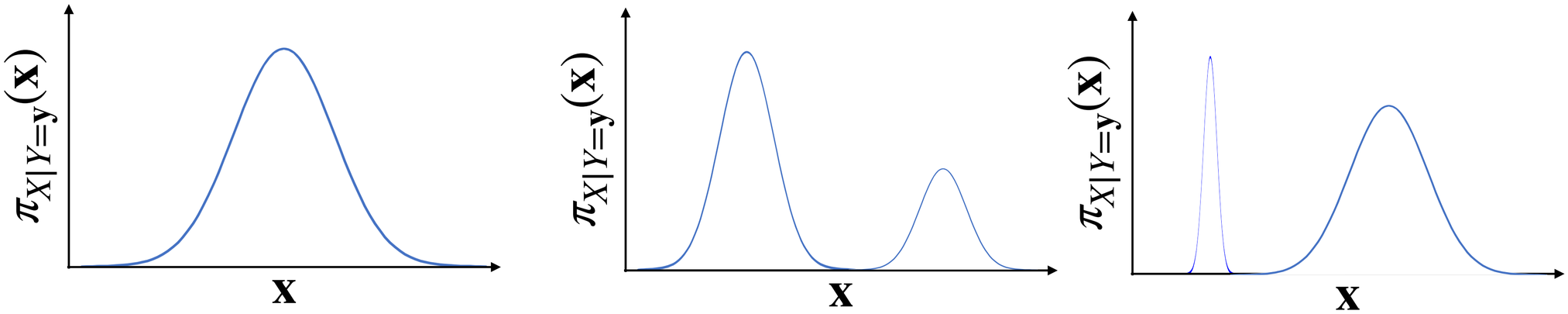
- This gives us the relation:

$$\pi_{X|Y=\mathbf{y}}(\mathbf{x}) = \frac{1}{c}\exp\left(-\frac{\|\mathbf{y} - F(\mathbf{x})\|_2^2}{2\sigma^2}\right)\exp\left(-\frac{\mathbf{x}^T\mathscr{C}^{-1}\mathbf{x}}{2}\right)$$

- The constant c is referred to as the normalization constant.

Point Estimations of the Posterior

- Now that we have a distribution $\pi_{X|Y=\mathbf{y}}$, what should we report as the solution to the inverse problem.
- Some examples of possible posterior distributions:



Point Estimations of the Posterior

- The maximum a posterior (MAP) estimation

$$\mathbf{x}_{\text{MAP}} := \arg\max_{\mathbf{x}} \quad \pi_{X|Y=\mathbf{y}}(\mathbf{x})$$

- The posterior mean (or sometimes conditional mean)

$$\mathbf{x}_{\text{mean}} := \mathbb{E}(X \,|\, Y = \mathbf{y}) = \int_{\Omega} \mathbf{x} \pi_{X|Y=\mathbf{y}}(\mathbf{x}) \; d\mathbf{x}$$

- However, there is no right or wrong point estimators!

Connection to the Tikhonov regularization

Exercise (HW1)

- For the inverse problem:

$$\mathbf{y} = F(\mathbf{x}) + \mathbf{e}$$

- A classic solution to inverse problems are Tikhonov regularized optimization:

$$\mathbf{x}_{\text{Tyk}} := \arg\min_{\mathbf{x}} \ \|F(\mathbf{x}) - \mathbf{y}\|_2^2 + \lambda \|\mathbf{x}\|_2^2$$

- Show that for the posterior

$$\pi_{X|Y=\mathbf{y}}(\mathbf{x}) = \frac{1}{c} \exp\left(-\frac{\|\mathbf{y} - F(\mathbf{x})\|_2^2}{2\sigma^2}\right) \exp\left(-\frac{\|\mathbf{x}\|_2^2}{2}\right),$$

  i.e., linear inverse problem with Gaussian noise and standard-normal prior ,i.e., $X \sim \mathcal{N}(0, I_n)$, we have

$$\mathbf{x}_{\text{Tik}} = \mathbf{x}_{\text{MAP}}$$

- What is the regularization parameter λ in this case?

Connection to the Tikhonov regularization

Exercise (HW1)

- Hints: Start with the MAP minimization problem.
- In the arg-min problem, you can take $\log$ of and/or multiply the argument with a positive constant without effecting its results.
- Same is true when dropping constants.
- When multiplying an arg-min problem with a negative value, the problem becomes arg-max, and vice-versa.

Markov chain Monte-Carlo

Sampling Complex distributions

Babak Maboudi - day 2 - Jyväskylä summer school 2025

Markov chains

Monte Carlo Integration

- Let X be an $\mathbb{R}^n$-valued random variable, i.e., a random variable which takes values in $\mathbb{R}^n$, and f be an integrable function. Then

$$\mathbb{E}(f(X)) = \int_{\mathbb{R}^n} f(\mathbf{x})\pi_X(\mathbf{x})\ d\mathbf{x} \approx \sum_{j=1}^{N} w_j f(\mathbf{x}_j),$$

- In Monte Carlo Integration, $\mathbf{x}_j$ are i.i.d. realization of π_X, then the approximator becomes the ergodic average:
  - Mean approximation

$$\mathbf{m} = \mathbb{E}(X) \approx \sum_{j=1}^{N} \frac{1}{N}\mathbf{x}_j$$

  - Variance approximation

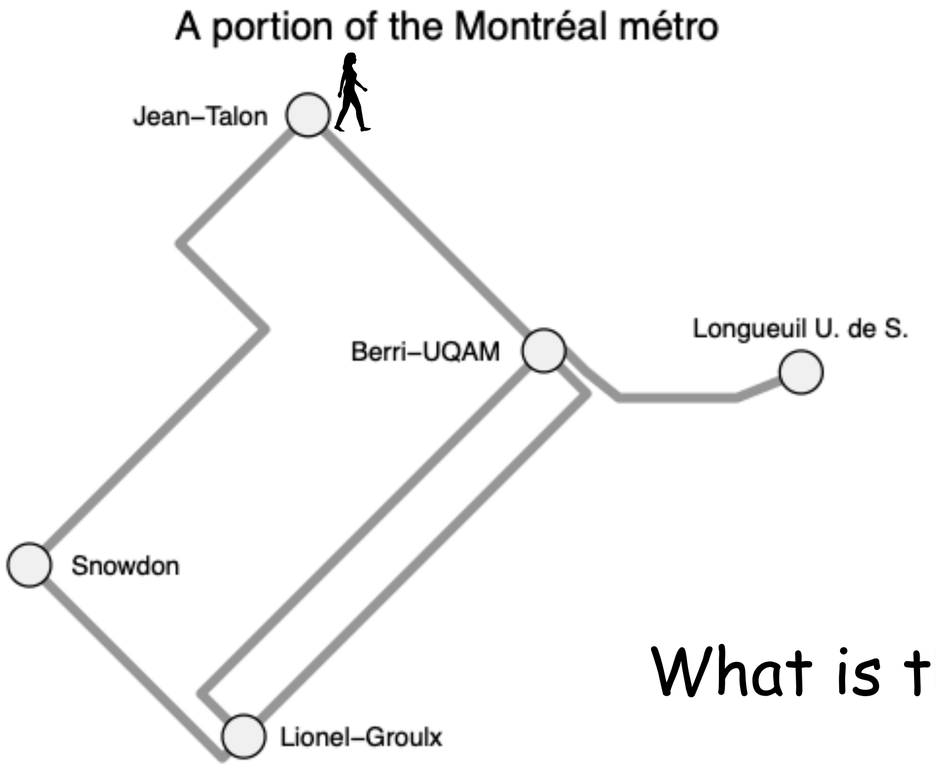
$$v = \mathrm{Var}(X) = \mathbb{E}(\|X - m\|_2^2) \approx \sum_{j=1}^{N} \frac{1}{N-1}\|\mathbf{x}_j - \mathbf{m}\|_2^2$$

Monte Carlo Integration

- However, the foundation for Monte Carlo estimation is independent realizations of the distribution of X.
- In Inverse Problems, we rarely have access to the distribution of X, this requires a complete knowledge of the density function.
- However, dependent sampling is possible! This is the principle idea of Markov-chain Monte Carlo methods.

Montréal Metro Map

Exercise from Art B. Owen (2013)



What is the distribution of

Alice's location?

Markov chains

Introducing notations

- Let $\Omega = \{\omega_1, \ldots, \omega_M\}$ be the *State Space*.
- Let X be a *Ω-valued random variable*.

Markov chains

Introducing notations

- Definition: A *Markov chain* is a sequence $X_0, X_1, X_2, \ldots, X_N$ (or $\{X_i\}_{i \leq N}$) of random variables with Markov property:
  - $\mathbb{P}(X_{i+1} \in A \,|\, X_j = x_j,\ 0 \leq j \leq i) = \mathbb{P}(X_{i+1} \in A \,|\, X_i = x_i)$
  - Here A is a set of states.
  - This is referred to being memoryless.

Markov chains

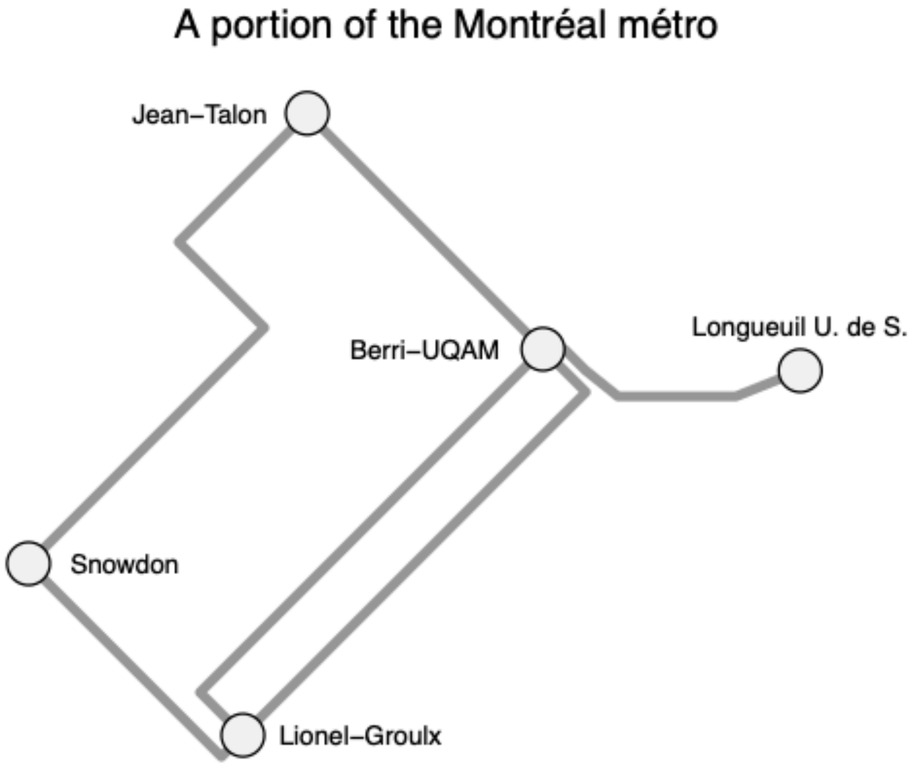
Further conditions

- A Markov chain is *(time-)homogeneous* if
$$\mathbb{P}(X_{i+1} = y \,|\, X_i = x) = \mathbb{P}(X_1 = y \in A \,|\, X_0 = x)$$
- A *transition probability* is the probability of going from state ω_i to ω_j:
$$p_{i \leftarrow j} = p_{ij} = \mathbb{P}(X_1 = \omega_i \in A \,|\, X_0 = \omega_j)$$
- A *transition matrix* is when you collect all transition probabilities in a matrix.
$$P = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1M} \\ p_{21} & p_{22} & \cdots & p_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ p_{1M} & p_{M2} & \cdots & p_{MM} \end{pmatrix}$$

Markov chains

Exercise 1 - `exercise_1.py`

- Choose a starting station
- Apply the function `roam` to move to the next station
- Draw 10000 samples from Montréal métro problem.
- Plot the histogram of the samples.
- Which station is the most likely destination?



Markov chains

Exercise 2 - `exercise_2.py`

- Now suppose that the initial state is not deterministic:
  $p_0(\omega_j)$: the probability of being at the jth station on the first step
- Similarly we define:
  $p_n(\omega_j)$: the probability of being at the jth station on the nth step
- What is the probability of being in the second station after 1 step?

$$p_1(\omega_2) = p_0(\omega_1)p_{21} + p_0(\omega_2)p_{22} + \ldots + p_0(\omega_M)p_{2M} = \sum_j p_{2j}p_0(\omega_j)$$

- Complete the python code `exercise_2.py` to compute $p_1(\omega_2)$ when you are initially at any given station with equal probability, i.e.,

$$p_0(\omega_j) = 1/5, \quad j = 1,\ldots,5,$$

- Can you write an operation between P and p_0 that gives you all the probabilities $p_1(\omega_j)$, for $j = 1,\ldots,5$?
- What is the sum of the elements in p_1? Why?

Markov chains

- We have

  $$p_1 = Pp_0,$$

  then,

  $$p_2 = Pp_1,$$

  and

  $$p_n = Pp_{n-1}.$$

- What is the transition matrix Q for doing 2 steps? i.e., what is the matrix Q that gives you:

  $$p_2 = Qp_0$$

  Hint: look at the Markovian principle (the recursive definitions above).

Markov chains

Exercise 3

- Compute the transition matrix, P^2, for 2 steps?
- Compute the transition matrix, P^{200}, for 200 steps?
- What does the pattern in P^{200} mean?
  Hint: the component $[P^{200}]_{ij}$, i.e., the element on the ith row and the jth column of P^{200}, means the probability of starting at the station j and after 200 steps of the Markov chain arriving at station i.

Sampling using a Markov chain

Explanation,

- What ever value X_0 has it will be almost forgotten (independent) in X_{100}.
- What ever value X_{100} has, it will be forgotten (independent) in X_{200}.
- If we take a widely separated sequence of equi-spaced samples we should get a nearly i.i.d. samples.
- Repeat the Markov chain sampling in `exercise_1.py`, but this time select only every 100 samples. Create a histogram and normalize it.
- Find the distribution p_{1000}, i.e., $P^{1000}p_0$. Compare the histogram with p_{1000}.

Markov Chain

Stationary distribution

- We say π is a stationary distribution when:

$$P\pi = \pi$$

  In other words, the transition matrix doesn't change the distribution.

Irreducible and periodic transition kernels

- What can you say about these transition matrices? Do they have a unique stationary distribution?

$$P_1 = \begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 1/2 & 1/2 \end{pmatrix}, \qquad P_1 = \begin{pmatrix} 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 1/2 & 1/2 \\ 1/2 & 1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \end{pmatrix}.$$

Irreducible and aperiodic transition kernels

- Theorem: If a transition matrix P is irreducible and aperiodic, and has a stationary distribution π then:

$$\lim_{n \to \infty} \mathbb{P}_{\omega_0}(X_n = \omega) = \pi(\omega)$$

- This “means” that the Markov chain method can arrive at the stationary distribution.

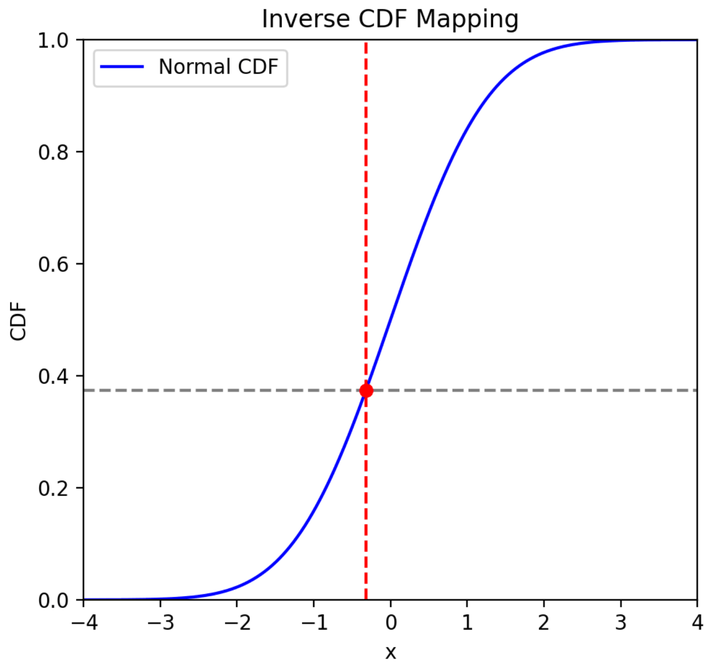
Veritasium video on Markov and Markov chains

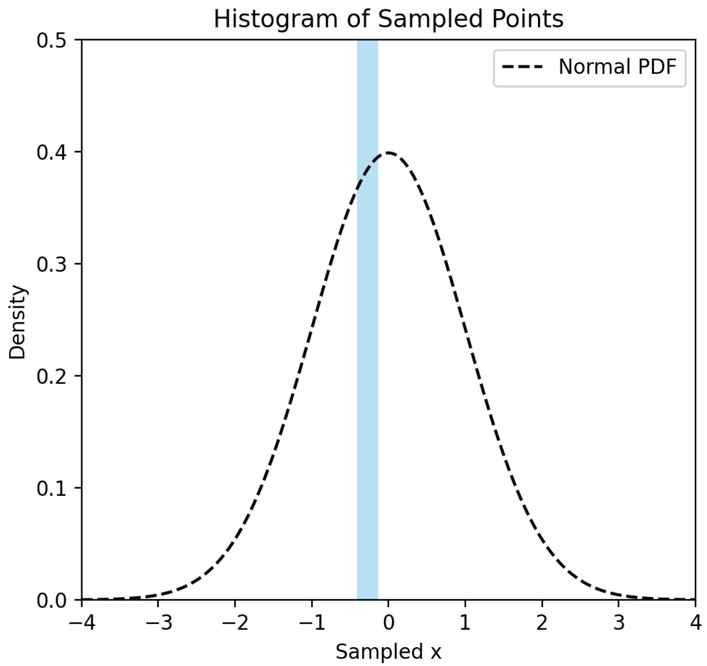
Acceptance/Rejection Sampling

Sampling from a Distribution

The inverse CDF method

$$F_X(x) = \mathbb{P}(X < x) = \int_{-\infty}^{x} \pi_X(x)\ dx$$



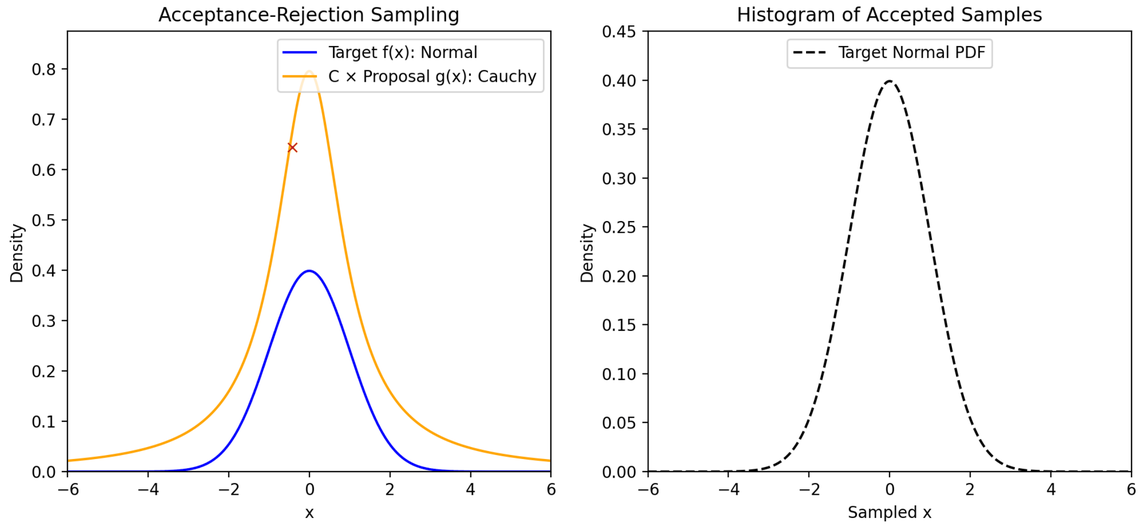


Sampling from a Distribution

Acceptance/Rejection method

- f is the density of the target distribution
- g is a density of a distribution that is easy t sample from (e.g. using the inverse CDF method).
- Algorithm:

    1. Sample y according to g
    2. Sample u according to $U(0,1)$
    3. If $u \leq f(y)/(Cg(y))$ accept, otherwise reject
    4. Repeat until desired samples achieved.



Acceptance/Rejection Sampling

Exercise (HW2)

- Get the Python script `exercise_4.py` from day 2 folder.
- Write Python functions `f(x)` and `g(x)` that computes the density functions of target Gaussian distribution and proposal Cauchy distribution:

$$f(x) = \frac{1}{\sqrt{(2\pi)}} \exp(-\frac{x^2}{2}), \qquad g(x) = \frac{1}{\pi(1+x^2)}$$

- Set $c = 2$ and perform acceptance/rejection to draw 2000 samples from the distribution of f, i.e.,
  - draw a sample $x^\star$ from the proposal distribution g.
  - Draw a number from the uniform distribution $u \sim U(0,1)$
  - If $cg(x)u \leq f(x)$ accept $x^\star$ as a sample from f, otherwise reject.
- Plot the histogram of the samples and show that they approximate a standard-normal distribution.
- Choose the "step-size" $c = 1, 1.52$, and 2 and repeat the sampling. Compute the number of accepted samples. Which value is the best and why?

Metropolis-Hastings Algorithm

Sampling from complex distributions

Babak Maboudi - day 3 - Jyväskylä summer school 2025

New notation

- From now on will consider continuous state space
  before: $\Omega = \{\omega_1, \ldots, \omega_M\}$ now $\Omega = [0,1]$ or $\mathbb{R}$
- Transition probability:
  before: $[P]_{ij} = p_{ij}$ now $P(y \leftarrow x)$
- Transition strategy:
  before: matrix now transition kernel
- We still may use sum for an easier visual interpretation (to avoid introducing differentials and probability measures)

Intention

- We want to find the transition matrix/kernel P that results in a stationary distribution π, where π is the posterior distribution of out inverse problem.
- Recall that the Bayes' rule indicates:

$$\pi_{X|Y=\mathbf{y}}(\mathbf{x}) = \frac{\pi_{Y|X=\mathbf{x}}(\mathbf{y})\pi_X(\mathbf{x})}{\pi_Y}(\mathbf{y}) \propto \pi_{Y|X=\mathbf{x}}(\mathbf{y})\pi_X(\mathbf{x})$$

  - $\pi_{X|Y}$ is the posterior
  - $\pi_{Y|X}$ is the likelihood
  - π_X is the prior distribution
  - $\pi_Y(\mathbf{y})$ is the data distribution, which is difficult to compute and is independent of X.

Detailed Balance

Exercise 1

- Recall that when arriving at the stationary distribution we will have

$$P\pi = \pi$$

  - Here, P is the transition matrix/kernel.
  - π is the stationary distribution.

- We want to design a P with a stationary distribution $\pi_{X|Y=\mathbf{y}}$.

Balance condition

- Recall that in a stationary distribution π of a transition probability matrix P we have that:

$$\sum_{\mathbf{x}\in\Omega} P(\mathbf{y}\leftarrow\mathbf{x})\pi(\mathbf{x}) = \pi(\mathbf{y})$$

$$= \int_{\Omega} P(\mathbf{y}\leftarrow\mathbf{x})\pi(\mathbf{y})\ d\mathbf{y}$$

- Now multiply right side with $1 = \sum_{x\in\Omega} P(\mathbf{x}\leftarrow\mathbf{y})$

$$\sum_{\mathbf{x}\in\Omega} P(\mathbf{y}\leftarrow\mathbf{x})\pi(\mathbf{x}) = \sum_{\mathbf{x}\in\Omega} P(\mathbf{x}\leftarrow\mathbf{y})\pi(\mathbf{y})$$

or

$$\sum_{\mathbf{x}\in\Omega,\mathbf{x}\neq\mathbf{y}} P(\mathbf{y}\leftarrow\mathbf{x})\pi(\mathbf{x}) = \sum_{\mathbf{x}\in\Omega,\mathbf{x}\neq\mathbf{y}} P(\mathbf{x}\leftarrow\mathbf{y})\pi(\mathbf{y})$$

Detailed Balance Condition

- Recall the balance condition:

$$\sum_{\mathbf{x}\in\Omega,\mathbf{x}\neq\mathbf{y}} P(\mathbf{y}\leftarrow\mathbf{x})\pi(\mathbf{x}) = \sum_{\mathbf{x}\in\Omega,\mathbf{x}\neq\mathbf{y}} P(\mathbf{x}\leftarrow\mathbf{y})\pi(\mathbf{y})$$

- A sufficient condition for balance condition is detailed balance condition:

$$P(\mathbf{y}\leftarrow\mathbf{x})\pi(\mathbf{x}) = P(\mathbf{x}\leftarrow\mathbf{y})\pi(\mathbf{y}), \quad \text{for all } \mathbf{x},\mathbf{y}\in\Omega$$

- We already have π (the posterior) how can we choose P?
- It would be very nice to choose any P that we want 😈😅

Metropolis-Hastings Acceptance Probability

- Let us design a transition matrix/kernel $Q(\mathbf{y} \leftarrow \mathbf{x})$ and plug-into the detailed balance relation:

$$Q(\mathbf{y} \leftarrow \mathbf{x})\pi(\mathbf{x}) \neq Q(\mathbf{x} \leftarrow \mathbf{y})\pi(\mathbf{y}),$$

- We can correct the imbalance using acceptance/rejection (Hastings) strategy:

$$A(\mathbf{y} \leftarrow \mathbf{x})Q(\mathbf{y} \leftarrow \mathbf{x})\pi(\mathbf{x}) = A(\mathbf{x} \leftarrow \mathbf{y})Q(\mathbf{x} \leftarrow \mathbf{y})\pi(\mathbf{y}),$$

  - We know π: the posterior
  - We know Q: generic (aperiodic, irreducible and time-reversible) transition kernel
  - We only need to know A: The probability of accepting $\mathbf{y}$ moving from $\mathbf{x}$.
  - All terms are ≤ 1

Metropolis-Hastings Acceptance ratio

- Let us reformulate the final equation

$$A(\mathbf{y} \leftarrow \mathbf{x}) = \frac{Q(\mathbf{y} \leftarrow \mathbf{x})\pi(\mathbf{y})}{Q(\mathbf{x} \leftarrow \mathbf{y})\pi(\mathbf{x})} A(\mathbf{x} \leftarrow \mathbf{y}),$$

- Without loss of generality we assume:

$$A(\mathbf{x} \leftarrow \mathbf{y}) = \lambda Q(\mathbf{x} \leftarrow \mathbf{y})\pi(\mathbf{x})$$

- Then

$$A(\mathbf{y} \leftarrow \mathbf{x}) = \lambda Q(\mathbf{y} \leftarrow \mathbf{x})\pi(\mathbf{y})$$

- So

$$\lambda \times \max\left\{Q(\mathbf{x} \leftarrow \mathbf{y})\pi(\mathbf{x}), Q(\mathbf{y} \leftarrow \mathbf{x})\pi(\mathbf{y})\right\} = 1$$

- Substituting into above:

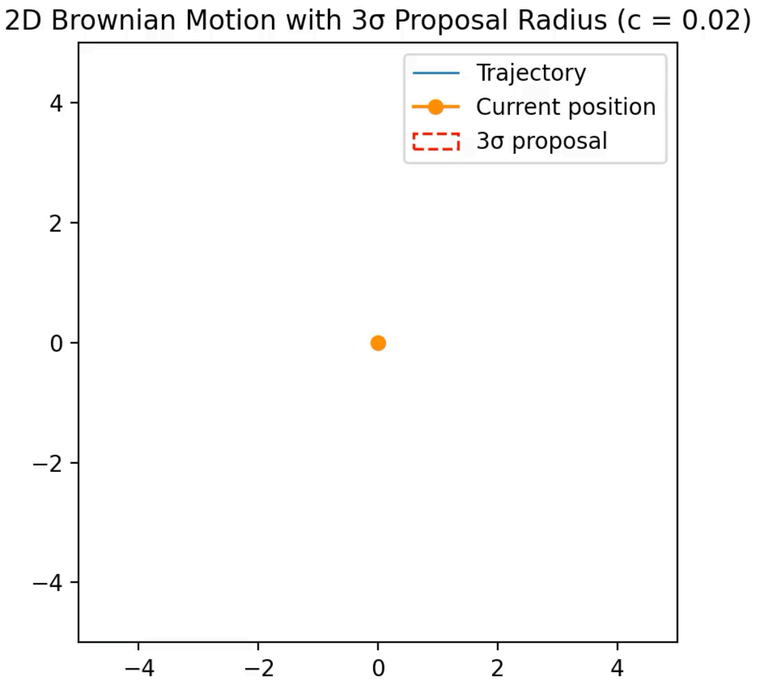
$$A(\mathbf{x} \leftarrow \mathbf{y}) = \min\left(1, \frac{Q(\mathbf{x} \leftarrow \mathbf{y})\pi(\mathbf{x})}{Q(\mathbf{y} \leftarrow \mathbf{x})\pi(\mathbf{y})}\right)$$

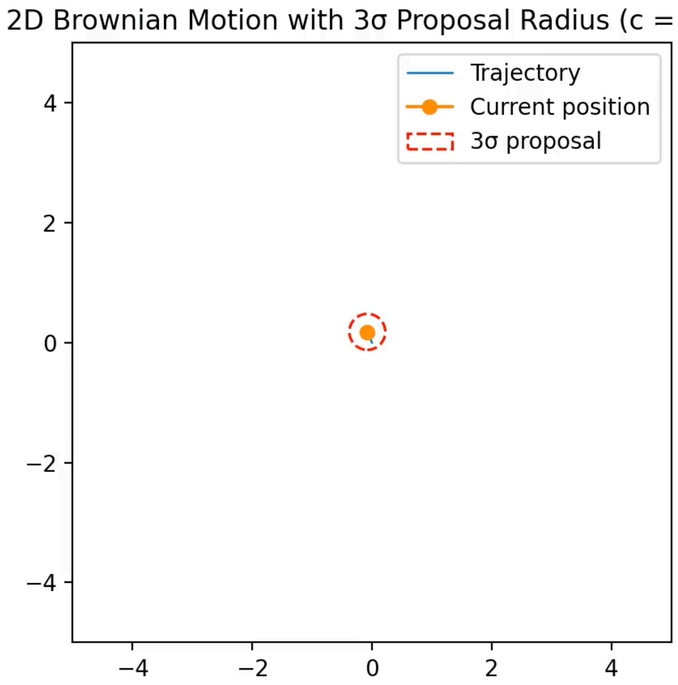
Random Walk Metropolis-Hastings algorithm

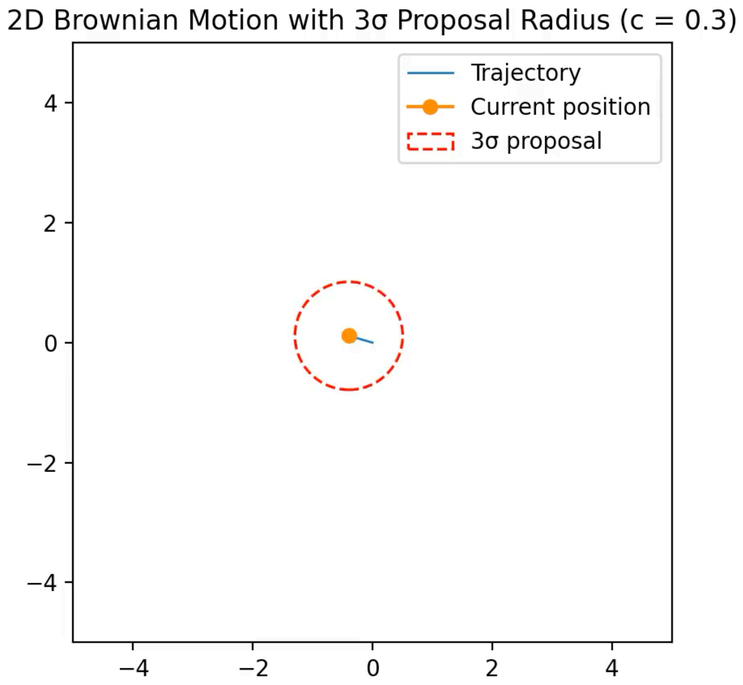
- Goal: To create a Markov chain with stationary distribution of the posterior distribution.
- Take a state $\mathbf{x}_0$ with probability $\pi(\mathbf{x}_0) \neq 0$ as you first element in your Markov chain, i.e.,
$$\mathbf{x} = \mathbf{x}_0$$
- Choose a transition kernel Q of your choice!
- Propose a new sample $y \sim Q_{\mathbf{x}}$.
- Form the Metropolis-Hasting acceptance ratio
$$a = \min\left(1, \frac{Q(\mathbf{x} \leftarrow \mathbf{y})\pi(\mathbf{x})}{Q(\mathbf{y} \leftarrow \mathbf{x})\pi(\mathbf{y})}\right)$$
- Draw a random number $u \sim U(0,1)$
- If $\alpha > u$ accept the proposal and set $x = y$, else reject the sample.
- Repeat until the desired samples are collected.

Example (most common) transition kernel

Brownian motion - a symmetric transition strategy







Your (probably) First Statistical Inversion

- Consider the inverse problem:

$$Y = \mathscr{A}X + E$$

  - $X \in \mathbb{R}^2$, $Y, E \in \mathbb{R}^3$ and

$$\mathscr{A} = \begin{pmatrix} 1 & -1 \\ 1 & -2 \\ 2 & 1 \end{pmatrix}.$$

  - Assume that

$$\pi_E(e) \propto \exp(-\frac{1}{2\sigma^2}\|e\|_2^2), \text{ with } \sigma^2 = 0.09.$$

  - Assume that the prior distribution for X is standard normal distribution, i.e.,

$$\pi_X(x) \propto \exp(-\frac{1}{2}\|x\|_2^2)$$

Your (probably) First Statistical Inversion

Exercise (HW3)

- Use the Bayes' theorem to write the density function of the posterior distribution, $\pi_{X|Y=\mathbf{y}}(\mathbf{x})$, up to proportionality constant,

$$\pi_{X|Y=\mathbf{y}}(\mathbf{x}) \propto \cdots$$

  i.e., drop terms that are not a function of $\mathbf{x}$.

Your (probably) First Statistical Inversion

Exercise (HW3)

- Get the Python code `exercise.py` for day 3.
- Write a Python function `prior` that computes the prior density $\pi_X(\mathbf{x})$ without the proportionality constant
- Write a Numpy matrix to define the matrix $\mathscr{A}$
- Use the noise standard deviation `sigma` and the measurement `y_obs` in the code

Your (probably) First Statistical Inversion

Exercise (HW3)

- Write a Python function `likelihood` that computes the likelihood density $\pi_{Y|X=\mathbf{x}}(\mathbf{y})$ without the proportionality constant. Here, $\mathbf{y}$ is `y_obs`.
- Write a Python function `posterior` that computes the posterior density $\pi_{Y|X=\mathbf{x}}(\mathbf{y})\pi_X(\mathbf{x})$ without the proportionality constant. Use `prior` and `likelihood` functions.

Your (probably) First Statistical Inversion

Exercise (HW3)

- Complete the code for the Metropolis-Hastings random walk algorithm:
  - Set the dimension of X
  - Choose an initial guess $\mathbf{x}$ for the Markov chain process
  - Choose a step size c for the Metropolis proposal. $c = 1$ is a good step size for this problem

Your (probably) First Statistical Inversion

Exercise (HW3)

- In the acceptance-rejection loop:
  - Choose a Gaussian proposal kernel. I.e., propose a point $x^\star$ according to
    $$\mathbf{x}^\star = \mathcal{N}(\mathbf{x}, c^2 I_2) \quad \text{or} \quad \mathbf{x}^\star = \mathbf{x} + c\mathbf{z}$$
    with $I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\mathbf{e} \sim \mathcal{N}(0, I_2)$
  - Compute the acceptance probability
    $$a = \min\left(1, \frac{\text{posterior}(\mathbf{x}^\star)}{\text{posterior}(\mathbf{x})}\right)$$
  - Draw a sample $u \sim U([0,1])$
  - Accept $\mathbf{x}^\star$ if $u < \alpha$ and set $\mathbf{x} = \mathbf{x}^\star$ and else reject the proposed sample.

Your (probably) First Statistical Inversion

Exercise (HW3)

- Draw 50000 samples from the posterior distribution with step size $c = 1$ in the random walk Metropolis-Hasting algorithm.
- Sub-sample (skip every 10) equi-spaced samples to achieve near i.i.d. samples of the posterio.
- Draw a 2D histogram of the posterior and mark the posterior mean on it.

Your (probably) First Statistical Inversion

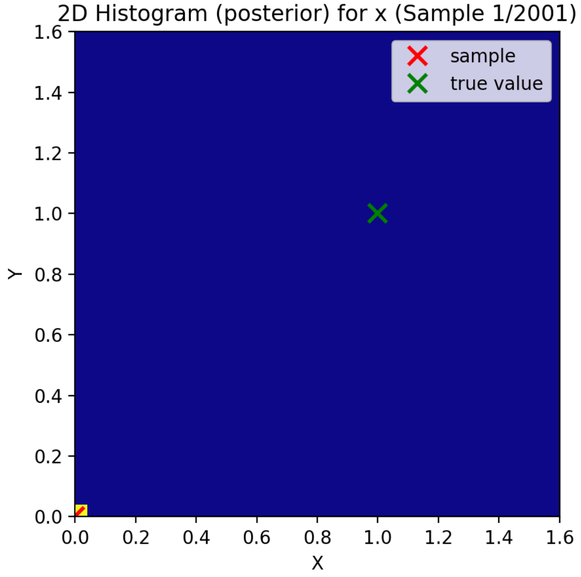
Exercise (HW3)

- Let the step-size $c \in \{0.001, 0.1, 10\}$. Plot the posterior 2D histogram for each step size and explain the differences. Which value of c is better for this problem, in your opinion, and why?

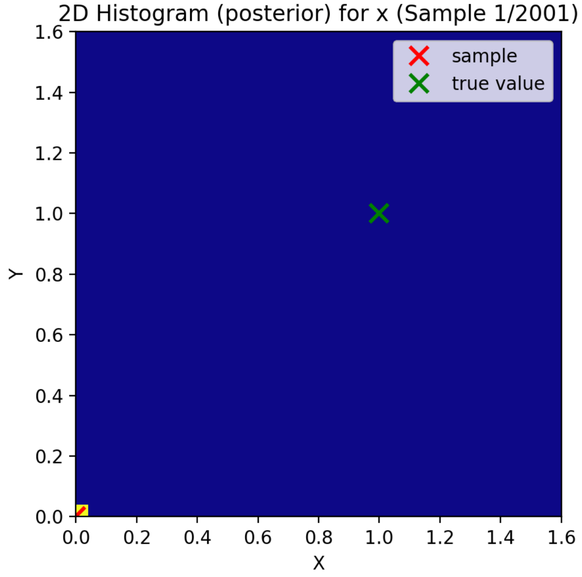
- Let noise variance be $\sigma^2 \in \{0.01, 0.1, 1\}$. Plot the posterior 2D histogram for each noise variance. What differences do you observe? Discuss uncertainty in the posterior mean estimation.

The effect of step size in random walk MH

$c = 0.01$



$c = 0.1$



$c = 1$