
Problem for Day 1. (optional) Consider the statistical inverse problem

$$Y = f(X) + E, \quad (1)$$

where $X \in \mathcal{N}(0, I_n)$, $E \sim \mathcal{N}(0, \sigma^2 I_m)$ where I_n and I_m are an $n \times n$ and $m \times m$ identity matrices, $\sigma > 0$ is the standard deviation of noise, and $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is the forward operator. Furthermore, we can write the probability density function of X and E as

$$\begin{aligned} \pi_X(\mathbf{x}) &= \frac{1}{\sqrt{(2\pi)^n}} \exp\left(-\frac{1}{2}\|\mathbf{x}\|_2^2\right), \\ \pi_E(\mathbf{e}) &= \frac{1}{\sqrt{(2\pi)^m \sigma^2}} \exp\left(-\frac{\|\mathbf{e}\|^2}{2\sigma^2}\right). \end{aligned}$$

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

$$\pi_{X|Y=\mathbf{y}} \propto \dots$$

Assume that f is smooth but not necessarily linear. Only express it in terms of f , \mathbf{x} , \mathbf{y} , and σ .

2. Show that the maximum a posteriori (MAP) estimate

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

is equivalent to the solution of a Tikhonov regularized optimization problem:

$$\mathbf{x}_{Tik} := \arg \min_{\mathbf{x}} \|f(\mathbf{x}) - \mathbf{y}\|_2^2 + \lambda \|\mathbf{x}\|^2,$$

for some $\lambda > 0$. Express λ in terms of σ .

Problem for Day 2. In this exercise we will sample from a standard normal distribution using the acceptance/rejection sampling method, based on the Cauchy proposal distribution. Consider the target density function (standard normal density function)

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

and the proposal density function (Cauchy density function)

$$g(x) = \frac{1}{\pi(x^2 + 1)}.$$

open the code `exercise_4.py` in day 2 folder and follow the following instructions.

1. write a Python functions $f(\mathbf{x})$ and $g(\mathbf{x})$ that computes the density functions of target Gaussian density f and proposal Cauchy density g .
2. set the step size $c = 2$ for acceptance/rejection algorithm and draw 2000 samples from the distribution of.
3. Plot the histogram of the samples and show that they approximate a standard-normal distribution.
4. Choose the step-size $c = \{1.152, 2\}$, and repeat the sampling. Compute the number of accepted samples. Which value is the best and why?

Problem for Day 3. Consider the statistical inverse problem

$$Y = \mathcal{A}X + E, \quad (2)$$

where $X \in \mathbb{R}^2$ and $Y \in \mathbb{R}^3$ are real-valued multivariate random variables and $\mathcal{A} \in \mathbb{R}^{3 \times 2}$ is a matrix given by

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

Further more, suppose that the prior X and noise E follow the distributions $X \sim \mathcal{N}(0, I_2)$ and $E \sim \mathcal{N}(0, \sigma^2 I_3)$, where I_2 and I_3 are the 2 and 3 dimensional identity matrix, respectively.

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

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

only express it in terms of \mathcal{A} , \mathbf{x} , \mathbf{y} , σ .

2. open the code `exercise.py` in day 3 folder and follow the following instructions
 - (a) write a function `prior` that computes the prior probability density of an input \mathbf{x} .
 - (b) define a Numpy matrix `A` that holds \mathcal{A} .
 - (c) write a functions `likelihood` and `posterior` that computes the likelihood probability density and posterior probability density for an input \mathbf{x} . Here use `sigma` and `y_obs` that is provided in the code.
 - (d) Complete the code for the Metropolis-Hastings random walk algorithm based on transition strategy

$$\mathbf{x}^* = \mathcal{N}(\mathbf{x}, c^2 I_2),$$

or equivalently

$$\mathbf{x}^* = \mathbf{x} + c\mathbf{z}.$$

Here, \mathbf{z} is a sample from $\mathcal{N}(0, I_2)$ and c is the step-size in the random walk Metropolis-Hastings algorithm.

3. Draw 50000 samples from the posterior distribution. Down-sample (skip every 10 samples) to create a near i.i.d. samples of the posterior. plot a 2D histogram of the posterior and mark the posterior mean on it.
4. Let the step size be $c \in \{0.001, 0.1, 10\}$. Plot the posterior 2D histogram for each step size and explain the differences. In your opinion, which value of c is better for this problem, and why?
5. 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.

Problem for Day 4. In this problem, we consider the statistical inverse problem of 1D de-blurring, formulated as

$$Y = \mathcal{A}X + E, \quad (3)$$

where X, Y and E are all random variables in \mathbb{R}^n , and $\mathcal{A} \in \mathbb{R}^{n \times n}$ is a blurring matrix. Complete the Python code `exercise_1.py` in day 4 folder following these instructions.

1. the vector \mathbf{s} contains a discretization of the interval $[0, 1]$ with step size $\Delta s = 1/100$. Use \mathbf{s} to create a vector \mathbf{x} that approximates the signal

$$x(s) = \begin{cases} 1, & 0.2 \leq s \leq 3.5, \\ 2, & 0.5 \leq s \leq 0.7, \\ 0 & \text{otherwise.} \end{cases}$$

2. Use the Python function `A` to add blurr to \mathbf{x} and create blurred measurement \mathbf{y} and add noise to create noisy measurement `y_obs`, using blurring standard deviation $\delta = 1$ (in the code this is defined by `delta`). Plot the original signal \mathbf{x} and the blurred measurements \mathbf{y} and noisy measurements `y_obs`.

Now we use the Bayes' theorem to construct the posterior as

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

and investigate different choices for the prior $\pi_X(\mathbf{x})$.

Uncorrelated prior: the first exercise is to choose the prior $\pi_X(\mathbf{x})$ to be

$$X \sim \mathcal{N}(0, I_n),$$

where I_n is the n -dimensional identity matrix. Continue completing the code following these instructions.

3. Write the density function of the posterior distribution up to the proportionality constant when $E \sim \mathcal{N}(0, \sigma^2 I_n)$, i.e.,

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

4. Complete the code in `exercise_2.py` using the steps below in order to enable sampling from the posterior distribution of this inverse problem:

(a) write a Python function `prior` that computes the log (un-normalized) prior density, i.e.,

$$\log \pi_X(\mathbf{x}) = -\frac{1}{2}\|\mathbf{x}\|_2^2$$

(b) write a Python function `likelihood` that computes the log (un-normalized) likelihood density, i.e.,

$$\log \pi_{Y|X=\mathbf{x}}(\mathbf{y}) = -\frac{1}{2\sigma^2}\|\mathbf{y} - \mathcal{A}\mathbf{x}\|_2^2$$

(c) write a Python function `posterior` that computes the log (un-normalized) posterior density.

(d) using the random-walk Metropolis-Hasting algorithm, draw 10000 samples. Choose the step size c that gives you about 23% acceptance rate.

5. plot the posterior mean.

6. plot the point-wise variance as a measure of uncertainty, i.e., limit your samples to a point, e.g., $s = i\Delta s$ for a particular i , now your samples are real-valued samples. You can compute the variance of these samples. Then repeat for all points in \mathbf{s} .

7. Where are the regions that has high(er) uncertainty.

Increment (correlated) prior: In this exercise we will set the prior on increments instead of pixel values. Let us first introduce the random variable for the increments:

$$\mathbf{z}_i = \mathbf{x}_{i+1} - \mathbf{x}_i, \quad i = 1, \dots, n-1,$$

and let \mathbf{z} be the vector that contains \mathbf{z}_i . Define the Matrix T that transforms \mathbf{z} into \mathbf{x} , i.e., $\mathbf{x} = T\mathbf{z}$

8. Write how the matrix T look like.

Now let Z be the random variable associate with the vector \mathbf{z} , with the prior density function $\pi_Z(\mathbf{z})$ (the exact density will be discussed below).

8. Reformulate the statistical de-blurring inverse problem using the change of variable $X = TZ$ and $\mathbf{x} = T\mathbf{z}$. (you need to reformulate the prior to be π_Z and the likelihood to be $\pi_{Y|Z}$)

Now we will investigate different types of priors for Z . We will use Gaussian prior, Laplace prior and Cauchy priors. Laplace and Cauchy priors will promote sparsity in jumps, i.e., we, a priori, expect fewer jumps in the signal.

8. In the Python code `exercise_3.py` for day 4, write 3 functions that can compute the log density function for the prior, once for the Gaussian $\mathcal{N}(0, \sigma_{\text{prior}}^2 I_n)$, $\sigma_{\text{prior}} = 0.1$,

$$\pi_Z(\mathbf{z}) \propto \exp\left(-\frac{\|\mathbf{z}\|_2^2}{2\sigma_{\text{prior}}^2}\right),$$

once for the Laplace prior $\text{Laplace}(0, b)$, zero mean and scaling $b = 0.05$

$$\pi_Z(\mathbf{z}) \propto \exp\left(-\frac{\|\mathbf{z}\|_1}{b}\right)$$

and Once for the Cauchy $\text{Cauchy}(0, \gamma)$, zero mean and scaling $\gamma = 0.005$.

$$\pi_Z(\mathbf{z}) \propto \prod_{i=1}^{n-1} \frac{1}{1 + \left(\frac{z_i^2}{\gamma^2}\right)}$$

Don't forget to take the log of the prior!!!

9. Repeat the sampling as with the uncorrelated case. For each of the choices of prior make sure that you set the step size in the Metropolis-Hastings method such that you achieve acceptance rate of about 23%. Plot the posterior mean and point-wise variance. Explain the differences with respect to the uncorrelated prior. Which of these priors are the most suitable for the problem and why?

Problem for Day 5. In this exercise we will create a smooth prior and use it to solve the hydraulic conductivity problem.

To create a smooth prior we use a covariance kernel $f : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ and define a covariance matrix \mathcal{C} . We can then use this covariance matrix to define a Gaussian random variable.

Use the code `exercise_1.py` in day 5 folder and follow the instructions below

1. create a discretization of the interval $[0, 1]$ as a vector \mathbf{s} and store it in a Python variable \mathbf{s} .
2. create a python function `gaussian_cov_func` to evaluate the Gaussian covariance kernel:

$$f(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{|\mathbf{x} - \mathbf{x}'|^2}{2\ell^2}\right)$$

with $\ell = 0.05$ the correlation length.

3. create a covariance matrix \mathcal{C} with elements:

$$[\mathcal{C}]_{ij} = f(\mathbf{s}_i, \mathbf{s}_j).$$

4. use `np.random.multivariate_normal` to draw 5 samples from $\mathcal{N}(0, \mathcal{C})$. Plot the samples.
5. repeat the experiment for $\ell = 0.2, 0.1$ and 0.05 . And plot the samples. How does ℓ effects the samples?

6. now repeat the experiment above with the exponential kernel:

$$f(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{|\mathbf{x} - \mathbf{x}'|}{\ell}\right)$$

How does the behavior of the samples change?

7. Often in inverse problems, it is preferred to work with independent samples. However, components of $\mathcal{N}(0, \mathcal{C})$ are inherently correlated. We can perform a change of variable and create a set of independent variables using the change of variables

$$X = \mathcal{C}^{1/2} Z \quad (4)$$

where X is the original random variable, $\mathcal{C}^{1/2}$ is the Cholesky factor of \mathcal{C} , and now, Z is a new variable with distribution $\mathcal{N}(0, I_n)$. For the Gaussian kernel above draw 5 samples by first drawing $Z \sim \mathcal{N}(0, I_n)$ and then multiplying them by the $\mathcal{C}^{1/2}$.

we will now use this prior to formulate the posterior distribution of the hydraulic imaging problem.

The code `hydraulic.py` contains the numerical approximation of the forward operator. You can follow the code `exercise_2.py` to see how you can pass a conductivity (the unknown \mathbf{x}) to create 5 pressure profiles for 5 number of injections. The code will return a matrix where the i -th row corresponds to the discrete pressure profile for i -th injection/measurement.

For the Hydraulic inverse problem we consider the statistical inverse problem:

$$Y_i = F_i(X) + E_i, \quad i = 1, \dots, 5 \quad (5)$$

where F_i is the forward operator of the i th injection (in the code, the `hydraulic.py` will perform all F_i simultaneously), And $E_i = \mathcal{N}(0, \sigma_i I_n)$, for $i = 1, \dots, 5$. Remember that the noise standard deviations σ_i are different for each measurement.

8. For a prior distribution $X \sim \mathcal{N}(0, \mathcal{C})$ write the posterior distribution, up to constant of proportionality, i.e.,

$$\pi_{X|Y_1=\mathbf{y}_1, \dots, Y_5=\mathbf{y}_5}(\mathbf{x}) \propto \dots \quad (6)$$

Hint: Use the fact that the 5 measurements are independent, and therefore,

$$\pi_{Y_1, \dots, Y_5|X}(\mathbf{y}_1, \dots, \mathbf{y}_5) = \pi_{Y_1|X}(\mathbf{y}_1) \cdots \pi_{Y_5|X}(\mathbf{y}_5).$$

9. Reformulate and rewrite the posterior using the change of variable (4), i.e.,

$$\pi_{Z|Y_1=\mathbf{y}_1, \dots, Y_5=\mathbf{y}_5} \propto \dots$$

Recall that in this case the prior distribution is simply

$$Z \sim \mathcal{N}(0, I_n)$$

10. One measurement data is given to you in the file `obs.pickle`. The Python code `exercise_3.py` will read this file and create 2 variables `y_obs` and `sigma` which will hold the measurements $\mathbf{y}_1, \dots, \mathbf{y}_5$ and the noise standard deviations $\sigma_1, \dots, \sigma_5$.

11. complete the code in `exercise_3.py` to sample the posterior. Plot the posterior mean and point-wise posterior variance. Where in the solution do you suspect that there is a sudden increase in porosity?

These are steps to complete `exercise_3.py`

- (a) create a discretization of the interval $[0, 1]$ in a vector \mathbf{s} with $N=100$ points.
 - (b) initiate the hydraulic class with N with the command
`hydraulic = hydraulic_class(N)` .
 - (c) Create a covariance matrix of the prior using a Gaussian covariance kernel with length scale 0.1, i.e., `length_scale=0.1`.
 - (d) create the Cholesky factor of the covariance matrix.
For part (c) and (d) you can copy the code from the previous exercise.
 - (e) create a Python function that evaluates the log of the un-normalized prior density $\pi_Z(\mathbf{z})$ (standard normal distribution).
 - (f) load the measurement file `obs.pickle`.
 - (g) create a Python function that evaluates the log of the un-normalized likelihood density.
 - (h) combine the two to create a Python function that evaluates the log of posterior.
 - (i) perform the random walk Metropolis-Hastings sampling method to draw sample 10000 samples from the posterior. The step size $c = 0.003$ is appropriate for this problem.
for (i) you can copy the code from the exercises in day 4.
 - (j) compute the mean and the point-wise variance.
12. **(optional)** what happens to uncertainty in estimation when pressure sensors are broken in half of the domain? You can simulate faulty pressure sensors by throwing away half of the output of `hydraulic.forward`, i.e., the forward operator becomes
`hydraulic_broken = lambda x: hydraulic.forward(x)[: , N/2:]`
similarly you should discard half of the measurements in `y_obs`, i.e.,
`y_obs_broken = y_obs[: , N/2:]`