exercise 1

having fun with least squares optimization

solutions due

until **October 28, 2025** at **23:59** via **ecampus**

general remarks

Your instructor is an avid proponent of open science and open education and therefore favors working with of open source software.

The coding exercises for this course are therefore to be solved using `Python` / `numpy` / `scipy` / `sympy` / `matplotlib` ... If you are not yet familiar with these popular components of the `Python` data science stack, this course provides an opportunity to gather corresponding experience because **implementations in other languages will not be accepted**.

The practical problems on this and future exercise sheets are altogether rather simple. If you don't have any ideas for how to solve them, just search the Web for clues or solutions.

In fact, we encourage you to ask modern AIs for assistance. In other words, you are allowed to tackle the exercises with the help of ChatGPT, Gemini, Grok, Claude, Qwen, or whatever model you prefer. If you do, then please report your experiences so that we can *all* learn how to navigate a world where thinking machines are becoming a reality ...

Moreover, **if you work with AI assistance, then please diligently verify the correctness of whatever the AI tells you.**

Remember that you have to achieve at least 50% of the exercise points to be eligible to the written exam at the end of the semester.

Your grades (and credits) for this course will be decided on the exam, but —once again— you have to succeed in the exercises to get there.

All your solutions have to be *satisfactory* to count as a success. Your code and results will be checked and need to be convincing.

If your solutions meet the above requirements and you can demonstrate that they work in practice, they are *satisfactory* solutions.

A *very good* solution (one that is rewarded full points) requires additional efforts especially w.r.t. to readability of your code. If your code is neither commented nor well structured, your solution is not good! The same holds for your discussion of your results: these should be concise and convincing and demonstrate that you understood what the respective task was all about. Striving for very good solutions should always be your goal!

task 1.1

beware of numerical instabilities

Note: Every student in every team should do this task because everybody needs to know about potential pitfalls when using digital computers to get numerical solutions to computational problems! **There are no points for this task** since we will closely guide you. Still, we urge you to work through the following as it reveals that mathematical theory and digital computing practice are not always well aligned. This is important to know for those who develop machine learning solutions for real world applications . . .

Consider the following least squares problem

$$\boldsymbol{w}_\star = \operatorname*{argmin}_{\boldsymbol{w}} \left\| \boldsymbol{X}^\intercal \boldsymbol{w} - \boldsymbol{y} \right\|^2 \tag{1}$$

for which matrix $\boldsymbol{X}^\intercal$ and vector $\boldsymbol{y}$ are given by

$$\boldsymbol{X}^\intercal = \begin{bmatrix} 1.00000 & -1.00000 \\ 0.00000 & 0.00001 \\ 0.00000 & 0.00000 \end{bmatrix} \quad \text{and} \quad \boldsymbol{y} = \begin{bmatrix} 0.00000 \\ 0.00001 \\ 0.00000 \end{bmatrix} . \tag{2}$$

This particular problem is perfectly solved by

$$\boldsymbol{w}_\star = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

because $\boldsymbol{X}^\intercal \boldsymbol{w}_\star = \boldsymbol{y}$ so that $\left\| \boldsymbol{X}^\intercal \boldsymbol{w}_\star - \boldsymbol{y} \right\|^2 = 0$ which is the smallest possible value our quadratic objective function can assume.

Solving the problem in (1) is easy because its ingredients are small enough for us to “see” the solution. In practice, problems rarely are this simple. However, we already know that we can solve least squares problems as

$$\boldsymbol{w}_\star = \left[\boldsymbol{X} \boldsymbol{X}^\intercal \right]^{-1} \boldsymbol{X} \boldsymbol{y} \, . \tag{3}$$

In other words, we know that we can solve least squares problems for any $\boldsymbol{X}^\intercal$ and $\boldsymbol{y}$ (of matching dimensions).

So what happens if we implement the algebraic solution in (3) to use a computer to solve the problem in (1) with the ingredients in (2)?

task 1.1.1

Run the following code snippet and marvel at the output it prodcues

```
import numpy as np
import numpy.linalg as la

matX = np.array([[ 1.00000, 0.00000, 0.00000],
                 [-1.00000, 0.00001, 0.00000]])
vecY = np.array( [ 0.00000, 0.00001, 0.00000] )

vecW = la.inv(matX @ matX.T) @ matX @ vecY
print ('pen-and-paper solution:', vecW)
```

Below, you will find further sub-tasks. Yet, to make sense of what these are about, we first need some background information . . .

background info

A matrix is called "tall" or "thin" if it has more rows than columns. Matrix $\boldsymbol{X}^\intercal \in \mathbb{R}^{r\times c}$ in (2) is such a matrix and therefore has a QR decomposition

$$\boldsymbol{X}^\intercal = \boldsymbol{Q}\boldsymbol{R}$$

such that

$\boldsymbol{Q} \in \mathbb{R}^{r\times r}$ is orthogonal
$\boldsymbol{R} \in \mathbb{R}^{r\times c}$ is upper triangular .

Since the $r - c$ bottom rows of an upper triangular matrix only contain 0s, we may partition the product $\boldsymbol{Q}\boldsymbol{R}$ as follows

$$\boldsymbol{Q}\boldsymbol{R} = \begin{bmatrix}\boldsymbol{Q}_1 & \boldsymbol{Q}_2\end{bmatrix}\begin{bmatrix}\boldsymbol{R}_1 \\ \boldsymbol{0}\end{bmatrix} = \boldsymbol{Q}_1\boldsymbol{R}_1$$

where the columns of $\boldsymbol{Q}_1 \in \mathbb{R}^{r\times c}$ are still orthogonal and $\boldsymbol{R}_1 \in \mathbb{R}^{c\times c}$ is still upper triangular.

Note: `numpy`'s `linalg` module provides a function `qr` whose default is to return $\boldsymbol{Q}_1$ and $\boldsymbol{R}_1$ rather than $\boldsymbol{Q}$ and $\boldsymbol{R}$.

Now, observe the following: if $\boldsymbol{X}^\intercal = \boldsymbol{Q}_1\boldsymbol{R}_1$ and the columns of $\boldsymbol{Q}_1$ are orthogonal, then

$$\begin{aligned}\boldsymbol{w}_\star = \left[\boldsymbol{X}\boldsymbol{X}^\intercal\right]^{-1}\boldsymbol{X}\boldsymbol{y} &= \left[\boldsymbol{R}_1^\intercal\boldsymbol{Q}_1^\intercal\boldsymbol{Q}_1\boldsymbol{R}_1\right]^{-1}\boldsymbol{R}_1^\intercal\boldsymbol{Q}_1^\intercal\boldsymbol{y} \\ &= \left[\boldsymbol{R}_1^\intercal\boldsymbol{R}_1\right]^{-1}\boldsymbol{R}_1^\intercal\boldsymbol{Q}_1^\intercal\boldsymbol{y} \\ &= \boldsymbol{R}_1^{-1}\boldsymbol{R}_1^{-\intercal}\boldsymbol{R}_1^\intercal\boldsymbol{Q}_1^\intercal\boldsymbol{y} \\ &= \boldsymbol{R}_1^{-1}\boldsymbol{Q}_1^\intercal\boldsymbol{y}\end{aligned}$$

Hence, we just found that $\boldsymbol{w}_\star = \boldsymbol{R}_1^{-1}\boldsymbol{Q}_1^\intercal \boldsymbol{y}$ for which we note that the inverse of an upper triangular matrix (if it exists) can be computed quickly and with high numerical robustness.

task 1.1.2

Implement `numpy` code to compute $\boldsymbol{w}_\star = \boldsymbol{R}_1^{-1}\boldsymbol{Q}_1^\intercal \boldsymbol{y}$ and look at the result.

task 1.1.3

Implement `numpy` code that uses the `linalg` function `lstsq` to compute $\boldsymbol{w}_\star$ and look at the result. What do you think: Does the special purpose function `lstsq` solve least square problems via equation (3) or not?

task 1.1.4

Think about the meaning behind all this. Here are a few questions to guide your thoughts:

- Are real numbers and their floating floating point representations the same thing?
- What does it mean to speak about machine precision w.r.t. floating point arithmetic?
- What do we have to keep in mind when working with very large and very small floating point numbers?
- What do you find when you use pen and paper to compute the entries of $\boldsymbol{X}\boldsymbol{X}^\intercal$?
- what do you find when you use your computer to compute the entries of $\boldsymbol{X}\boldsymbol{X}^\intercal$?
- Can you blindly trust any piece of numerical software that some dude from somewhere has uploaded to github or even to huggingface?

task 1.2 [15 points]

cellular automata, the Boolean Fourier transform, and LSQ

In the lectures, we encountered the idea of feature maps which transform lower dimensional data to higher dimensional representations. Here, we explore this idea in a somewhat unusual context ...

background info

A one-dimensional (or elemental) cellular automaton consists of two basic components, namely

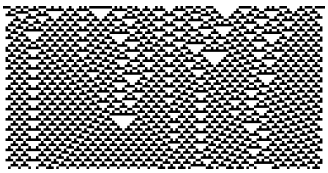
1) an infinite sequence of cells $\{x_j\}_{j\in\mathbb{Z}}$ each of which is in either one of two states, namely *off* or *on* which are usually encoded as $x_j \in \{0, 1\}$
2) an update rule $f : \{0, 1\}^3 \to \{0, 1\}$ for how to update a cell based on its and its two neighbors' current states

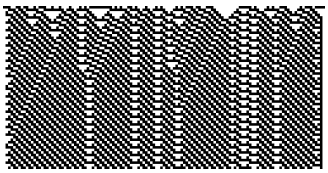
$$x_j[t+1] = f\Big(x_{j-1}[t], x_j[t], x_{j+1}[t]\Big) \ .$$

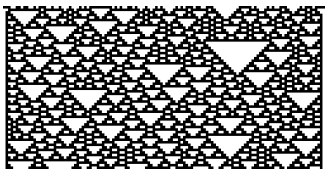
At time $t = 0$, the x_j are (randomly) initialized, and, at any (discrete) time step t, all cells are updated simultaneously. Here is an illustrative example where we plot 0 as □ and 1 as ■

t ···□□□□□□□□□□□□□□□□■□□□□□□□□□□□□□□□□···
$t+1$ ···□□□□□□□□□□□□□□□□■□■□□□□□□□□□□□□□□□□···

This update process continues forever and it is common to plot subsequent (finitely sized) state sequences below one another to visualize the evolution of an automaton under a certain rule. Here are some examples of possible evolutions all starting from the same initial configuration


rule 108


rule 110


rule 126

Henceforth, we will reduce notational clutter. That is, instead of writing

$$x_j[t+1] = f\Big(x_{j-1}[t], x_j[t], x_{j+1}[t]\Big)$$

we henceforth simply write

$$y = f(\boldsymbol{x})$$

where $\boldsymbol{x} \in \{0,1\}^3$ and $y \in \{0,1\}$.

The naming convention for the rules which govern the evolution of elemental cellular automata is due to **Stephen Wolfram** and illustrated in the following tables:

$\boldsymbol{X}^\intercal$			$\boldsymbol{y}$
0	0	0	0
0	0	1	1
0	1	0	1
0	1	1	1
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	0

rule 110

$\boldsymbol{X}^\intercal$			$\boldsymbol{y}$
0	0	0	0
0	0	1	1
0	1	0	1
0	1	1	1
1	0	0	1
1	0	1	1
1	1	0	1
1	1	1	0

rule 126

For $\boldsymbol{x} \in \{0,1\}^3$, there are $2^3 = 8$ possible inputs for each rule. For each input, there are 2 possible outputs. Hence, the total number of possible rules is $2^{2^3} = 256$.

We may collect the possible input patterns in an 8×3 matrix $\boldsymbol{X}^\intercal$ and the outputs of each rule in an 8 dimensional target vector $\boldsymbol{y}$. Converting a rule's binary target vector (read from bottom to top) into a decimal number then gives the rule's name.

Now, consider a seemingly crazy idea, namely the following substitution

$$\begin{aligned} 0 &\to +1 \\ 1 &\to -1 \,. \end{aligned}$$

People like this representation of binary states because there is a simple mapping from the ordered set $\{0, 1\}$ to the ordered set $\{+1, -1\}$, namely

$$x \in \{0, 1\} \quad \mapsto \quad x' = (-1)^x \in \{+1, -1\}$$

We can therefore convert binary functions $f_{01} : \{0, 1\}^n \to \{0, 1\}$ into bipolar functions $f_{+-} : \{+1, -1\}^n \to \{+1, -1\}$ by letting

$$f_{+-}\big((-1)^{x_1}, \ldots, (-1)^{x_n}\big) = (-1)^{f_{01}(x_1,\ldots,x_n)} \, .$$

Seen from this point of view, the above two tables representing rule 110 and rule 126 will look like this:

$\boldsymbol{X}^\intercal$			$\boldsymbol{y}$
$+1$	$+1$	$+1$	$+1$
$+1$	$+1$	-1	-1
$+1$	-1	$+1$	-1
$+1$	-1	-1	-1
-1	$+1$	$+1$	$+1$
-1	$+1$	-1	-1
-1	-1	$+1$	-1
-1	-1	-1	$+1$

rule 110

$\boldsymbol{X}^\intercal$			$\boldsymbol{y}$
$+1$	$+1$	$+1$	$+1$
$+1$	$+1$	-1	-1
$+1$	-1	$+1$	-1
$+1$	-1	-1	-1
-1	$+1$	$+1$	-1
-1	$+1$	-1	-1
-1	-1	$+1$	-1
-1	-1	-1	$+1$

rule 126

task 1.2.1 [5 points]

Given a matrix $\boldsymbol{X}^\intercal$ and a vector $\boldsymbol{y}$ as in the two tables above, implement `numpy` code that first solves the least squares problem

$$\boldsymbol{w}_\star = \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^3} \big\| \boldsymbol{X}^\intercal \boldsymbol{w} - \boldsymbol{y} \big\|^2$$

and then computes

$$\hat{\boldsymbol{y}} = \boldsymbol{X}^\intercal \boldsymbol{w}_\star \, .$$

Run your code for rules 110 and 126 and print the respective vectors $\boldsymbol{y}$ and $\hat{\boldsymbol{y}}$. Discuss what you observe.

Note: Don't be alarmed if your results seem less than optimal! What you are supposed to do here hardly makes any sense and is mainly intended as a preparation for what comes next. (Can you see *why* what you are supposed to do here hardly makes sense?) But before we move on, we need more background information.

more background info

A Boolean domain $\mathbb{B}$ is a set of exactly two numbers which represent the two truth values `false` and `true`. The most common examples of such domains are $\mathbb{B} = \{0, 1\}$ and $\mathbb{B} = \{-1, +1\}$.

Given this definition, it isn't a surprise that functions of the following form

$$f : \mathbb{B}^n \to \mathbb{B}$$

are called Boolean functions. Moreover, functions of the more general form

$$f : \mathbb{B}^n \to \mathbb{R}$$

are called pseudo Boolean functions and we note that, for $\mathbb{B} \subset \mathbb{R}$, the set of pseudo Boolean functions includes the set of Boolean functions.

Above, we already saw that each possible rule $y = f(\boldsymbol{x})$ which may govern the behavior of an elemental cellular automaton can be expressed as a (pseudo) Boolean function

$$f : \{\pm 1\}^n \to \{\pm 1\} \tag{4}$$

where $n = 3$. In what follows, we let $\mathcal{I}$ denote the index set of the entries x_j of $\boldsymbol{x} \in \mathbb{B}^n$, that is

$$\mathcal{I} = \big\{1, 2, \ldots, n\big\} \ .$$

The power set $2^{\mathcal{I}}$ of $\mathcal{I}$ is the set of all subsets of $\mathcal{I}$. In other words, we have

$$2^{\mathcal{I}} = \big\{\varnothing, \{1\}, \{2\}, \ldots, \{1, 2\}, \ldots, \{1, 2, \ldots, n\}\big\}$$

and we note that $\big|2^{\mathcal{I}}\big| = 2^n$.

Given these prerequisites, here is why Boolean functions as in (4) are interesting: "One can show" that every pseudo Boolean function

$$f : \{\pm 1\}^n \to \mathbb{R}$$

(and therefore every Boolean function of the form in (4)) can be uniquely expressed as a multilinear polynomial

$$f(\boldsymbol{x}) = \sum_{\mathcal{S} \in 2^{\mathcal{I}}} w_{\mathcal{S}} \prod_{j \in \mathcal{S}} x_j \ . \tag{5}$$

The expression in (5) is known as the Boolean Fourier series expansion of function f. In contrast to the complex exponentials which form the basis functions for conventional Fourier analysis, here the basis functions are the parity functions

$$\varphi_{\mathcal{S}}(\boldsymbol{x}) = \prod_{j \in \mathcal{S}} x_j$$

where by definition

$$\varphi_{\varnothing}(\boldsymbol{x}) = \prod_{j \in \varnothing} x_j = 1 \ .$$

Given these definitions of the $\varphi_{\mathcal{S}}(\boldsymbol{x})$, we can rewrite equation (5) as follows

$$f(\boldsymbol{x}) = \sum_{\mathcal{S} \in 2^{\mathcal{I}}} w_{\mathcal{S}} \, \varphi_{\mathcal{S}}(\boldsymbol{x}) = \boldsymbol{w}^{\mathsf{T}} \boldsymbol{\varphi}(\boldsymbol{x}) \tag{6}$$

This is interesting, because we now recognize that any (pseudo) Boolean function of the kind we are currently dealing with is an inner product of two high-dimensional vectors, namely

$$\boldsymbol{w} \in \mathbb{R}^{2^n}$$

and

$$\boldsymbol{\varphi}(\boldsymbol{x}) \in \{+1, -1\}^{2^n} \ .$$

task 1.2.2 [5 points]

Implement a `Python` / `numpy` function that realizes the transformation

$$\varphi : \{+1, -1\}^n \to \{+1, -1\}^{2^n}$$

which we implicitly introduced above.

To be specific, for an input vector $\boldsymbol{x} = [x_1, x_2, x_3]^\intercal \in \{+1, -1\}^3$, your code should produce the output vector

$$\varphi(\boldsymbol{x}) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_3 \\ x_1\,x_2 \\ x_1\,x_3 \\ x_2\,x_3 \\ x_1\,x_2\,x_3 \end{bmatrix} .$$

However, try to implement you function in a more general manner. That is, implement it such that it works for arbitrary $n \in \mathbb{N}$ rather than just for $n = 3$.

Tip: The `Python` standard library contains the module `itertools` which in turn provides functionalities that may come in handy for this task.

task 1.2.3 [5 points]

If we finally reconsider the matrices $\boldsymbol{X}^\intercal$ in the two tables you used above, we may think of them as row matrices

$$\boldsymbol{X}^\intercal = \begin{bmatrix} — & \boldsymbol{x}_0^\intercal & — \\ — & \boldsymbol{x}_1^\intercal & — \\ & \vdots & \\ — & \boldsymbol{x}_7^\intercal & — \end{bmatrix}$$

where

$$\boldsymbol{x}_0 = \begin{bmatrix} +1 \\ +1 \\ +1 \end{bmatrix} \qquad \boldsymbol{x}_1 = \begin{bmatrix} +1 \\ +1 \\ -1 \end{bmatrix} \qquad \ldots \qquad \boldsymbol{x}_7 = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix} .$$

Given your code from task 1.2.2, you should thus be able to compute a row matrix

$$\boldsymbol{\Phi}^\intercal = \begin{bmatrix} — \ \boldsymbol{\varphi}_0^\intercal \ — \\ — \ \boldsymbol{\varphi}_1^\intercal \ — \\ \vdots \\ — \ \boldsymbol{\varphi}_7^\intercal \ — \end{bmatrix}$$

where

$$\boldsymbol{\varphi}_j = \boldsymbol{\varphi}\big(\boldsymbol{x}_j\big) \ .$$

Given matrix $\boldsymbol{\Phi}^\intercal$ and the target vector $\boldsymbol{y}$ of a cellular automaton rule, write `Python` / `numpy` code that first solves the least squares problem

$$\boldsymbol{w}_\star = \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^8} \big\| \boldsymbol{\Phi}^\intercal \boldsymbol{w} - \boldsymbol{y} \big\|^2$$

and then computes

$$\hat{\boldsymbol{y}} = \boldsymbol{\Phi}^\intercal \boldsymbol{w}_\star \ .$$

Run your code for rules 110 and 126 and print the respective vectors $\boldsymbol{y}$ and $\hat{\boldsymbol{y}}$. What do you observe in comparison to your results in task 1.2.1?

What is the “price” you had to pay to obtain these (hopefully) much more reasonable results? Discuss this in your own words.

task 1.3 [15 points]

estimating the fractal dimension of objects in images

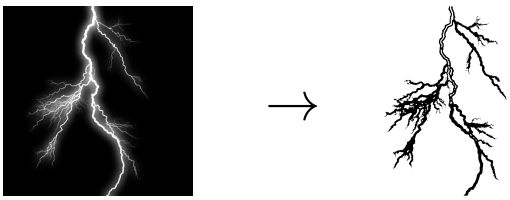
In our lectures, we discussed the use of least squares for linear regression. In this task, we consider a neat practical application of this technique.

background info

Box counting is a method for estimating the fractal dimension of an object in an image. For simplicity, we focus on square images whose width w and height h (in pixels) are integer powers of 2. For instance, if $w = h = 512$, then $w = h = 2^L$ where $L = 9$.

Given an image like this, the box counting procedure involves three steps:

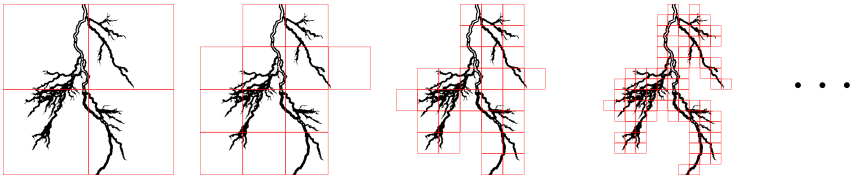
1. apply an appropriate binarization procedure to create a binary image in which foreground pixels are set to 1 and background pixels to 0



2. specify a set S of scaling factors $0 < s_l < 1$, for instance

$$S = \left\{ s_l = \tfrac{1}{2^l} \;\middle|\; l \in \{1, 2, \ldots, L-2\} \right\}$$

and, for each $s_l \in S$, cover the binarized image with boxes of size $s_l\, w \times s_l\, h$ and count the number n_l of boxes which contain at least one foreground pixel

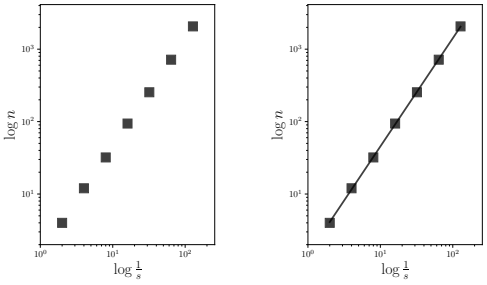


$s_l = \frac{1}{2}, n_l = 4$ $s_l = \frac{1}{4}, n_l = 12$ $s_l = \frac{1}{8}, n_l = 32$ $s_l = \frac{1}{16}, n_l = 94$

3. plot $\ln n_l$ against $\ln \frac{1}{s_l}$ and fit a line

$$D \cdot \ln \frac{1}{s_l} + b = \ln n_l$$

the resulting estimate for the slope D of this line represents the fractal dimension we are after. Here is an example for how such a line may look like:



In other words, the problem of estimating D is a simple linear regression problem that can of course be tackled using least squares.

here is your task

Implement `Python` / `numpy` / `matplotlib` code for the box counting method and run it on the images `tree.png` and `lightning.png`.

Which fractal dimensions do you obtain? Which object has the higher one, the tree or the lightning bolt?

Tip: We strongly suggest to work with the following imports

```
import numpy as np
import imageio.v3 as iio
import numpy.linalg as la
import scipy.ndimage as img
```

Tip: To read, say, image `tree.png` into a `numpy` array, you can then use

```
imgG = iio.imread('tree.png', mode='L').astype(float)
```

Note: While we do not really care about how you realize image I/O, we do care about how you binarize the images you read.

This is because after binarization, the outcome of the box counting procedure should be deterministic, i.e. the same for every team of exercising students. In other words, if every team uses the same binarization procedure, every team should obtain the same results and these results should be those your instructors got (up to numerical precision). Teams getting different results can rest assured they made a mistake.

Therefore, please use the following snippet

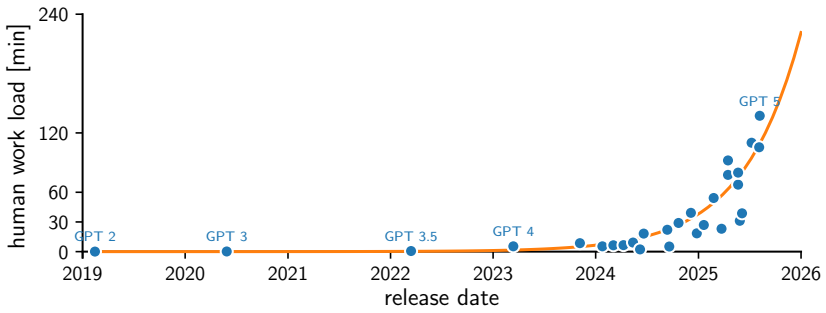
```
def binarize(imgF):
    imgB = np.abs(img.gaussian_filter(imgF, sigma=0.50) - \
                  img.gaussian_filter(imgF, sigma=1.00))

    return img.binary_closing(np.where(imgB < 0.1*imgB.max(), 0, 1))
```

task 1.4 [10 points]

fitting exponential models

In lecture 00, we discussed the following chart



which shows data points $(x_j, y_j) \in \mathbb{R} \times \mathbb{R}$ which have been gathered by the METR Institute together with an exponential model

$$y = f\big(x \;\big|\; A, B\big) = A \cdot \exp\big(B \cdot x\big) \tag{7}$$

which your instructor fitted to this data, i.e. for which he estimated suitable parameters A and B.

In this task, you will have the opportunity to (re-)create this fit by yourself. To this end, we first of all suggest you work with the following imports

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

Second of all, we made your task as "easy" as possible by extracting the METR data from its native `json` format into a `csv` file appropriately named `metrData.csv`. To read this file from disk, we suggest you use

```
df = pd.read_csv('metrData.csv')
```

where `df` is a `pandas` DataFrame which tabulates the relevant METR data. To look at the content of this table, you may simply `print(df)`. To extract the (x_j, y_j) data we are interested in, we finally suggest you read them into `numpy` arrays like so

```
xs = np.array(df['day'])
ys = np.array(df['est'])
```

background info

From task 1.1, you already know that numerical imprecision (due to under- or overflows) can cause problems in computational model fitting. When working with exponential models whose outputs grow rapidly, this must definitely be taken into consideration. Hence, to fit an exponential

$$y = A\,\exp\bigl(B\,x\bigr)$$

it is preferrable and common practice to take the logarithm of both sides

$$\ln y = \ln A + B\,x$$

in order to estimate the values $a = \ln A$ and B. Once these are available, the originally sought after model can be computed as $y = \exp\bigl(a + B\,x\bigr)$.

task 1.4.1 [5 points]

Implement code which solves the following *naïve* least squares problem

$$a_\star, B_\star = \operatorname*{argmin}_{a,B} \sum_j \bigl(\ln y_j - a - B\,x_j\bigr)^2 \tag{8}$$

and use it to fit an exponential model to the METR data. Plot the data and your fitted model and ponder what you observe.

Note: Your plot must be reasonable but does not have to look as fancy as the chart on the previous page.

task 1.4.2 [5 points]

The issue with the *naïve* least squares loss in (8) is that it puts too much emphasis on small y values. Using fancy terms, machine learners would say that (8) is a *biased* loss function (w.r.t. our current problem) as it too

eagerly *penalizes* large y values (which are of course quite important in our current setting).

Thus, in order to weight large y values more equally, it is better to minimize the following *robust* or *weighted* least squares loss

$$a_\star, B_\star = \operatorname*{argmin}_{a,B} \sum_j y_j \cdot \big(\ln y_j - a - B\, x_j\big)^2 \tag{9}$$

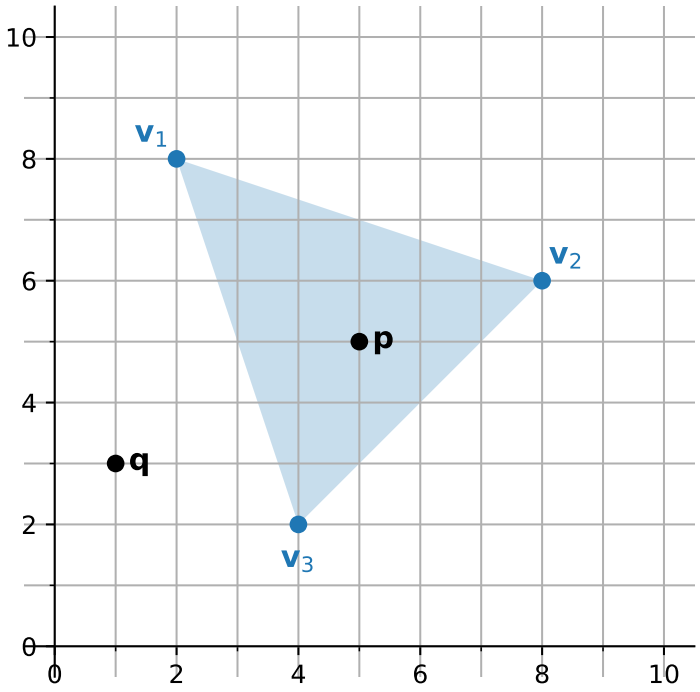
Implement code which solves this problem and then use your code to fit an exponential model to the METR data. Plot the data and your fitted model and ponder what you observe, i.e. compare your results for this sub-task to what you got in the previous sub-task.

Note: Again, your plot must be reasonable but does not have to look as fancy as the chart shown two pages ago.

task 1.5 [10 points]

barycentric coordinates

The following figure shows a triangle $\Delta(\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3)$ with vertices $\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3$ and two additional points $\boldsymbol{p}$ and $\boldsymbol{q}$ all residing in the Euclidean plane $\mathbb{R}^2$.



Recall that every point $\boldsymbol{p}$ *within* a triangle $\Delta(\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3)$ can be written as a *convex combination* of the vertices of said triangle

$$\boldsymbol{p} = \sum_{j=1}^{3} \boldsymbol{v}_j \cdot w_j \tag{10}$$

where the *barycentric coordinates* $w_j \in \mathbb{R}$ obey the *constraint equations*

$$\forall\, j : w_j \geq 0 \tag{11}$$

$$\sum_{j=1}^{3} w_j = 1\ . \tag{12}$$

Since convexity constraints like these will feature prominently later in this course, we might as well get used to them right now. In particular, we note

that we may write equations (11) and (12) much more compactly, namely

$$\boldsymbol{w} \succeq \mathbf{0} \tag{13}$$
$$\mathbf{1}^\intercal \boldsymbol{w} = 1 \tag{14}$$

where $\boldsymbol{w} = [w_1, w_2, w_3]^\intercal \in \mathbb{R}^3$ and $\mathbf{0}, \mathbf{1} \in \mathbb{R}^3$ denote the vectors of all zeros and all ones, respectively.

Having introduced vector $\boldsymbol{w}$, we can use it to write (10) more compactly, too. To this end, we also need the matrix

$$\boldsymbol{V} = \begin{bmatrix} | & | & | \\ \boldsymbol{v}_1 & \boldsymbol{v}_2 & \boldsymbol{v}_3 \\ | & | & | \end{bmatrix} \in \mathbb{R}^{2\times 3}$$

so that we can equivalently write (10) as

$$\boldsymbol{V}\,\boldsymbol{w} = \boldsymbol{p}\,. \tag{15}$$

Next, note that many blogs or other Web resources suggest to determine the barycentric coordinates $\boldsymbol{w}$ of $\boldsymbol{p}$ via Cramer's rule and determinant computations. But this is not how we roll in these exercises! Instead, we want you to estimate $\boldsymbol{w}$ via least squares optimization.

The "difficulty" is that, when we solve (15) for $\boldsymbol{w}$, we must make sure that the solution obeys the sum-to-one constraint in (14). To this end, we introduce even further objects, namely the following matrix and vector

$$\boldsymbol{X} = \begin{bmatrix} \boldsymbol{v}_1 & \boldsymbol{v}_2 & \boldsymbol{v}_3 \\ 1 & 1 & 1 \end{bmatrix} \in \mathbb{R}^{3\times 3} \qquad \text{and} \qquad \boldsymbol{y}_{\boldsymbol{p}} = \begin{bmatrix} \boldsymbol{p} \\ 1 \end{bmatrix} \in \mathbb{R}^3\,.$$

task 1.5.1 [2 points]

Letting $\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3$ and $\boldsymbol{p}$ as in the figure above, implement code that solves

$$\boldsymbol{w}_\star = \operatorname*{argmin}_{\boldsymbol{w}} \left\| \boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}_{\boldsymbol{p}} \right\|^2$$

and have a look at your result.

Does your result agree with the required convexity constraints? Also, compare the value of $\boldsymbol{V}\boldsymbol{w}_\star$ to the value of $\boldsymbol{p}$. What do you observe?

Next, letting $\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3$ and $\boldsymbol{q}$ as in the figure above, implement code to solve

$$\boldsymbol{w}_\star = \underset{\boldsymbol{w}}{\operatorname{argmin}} \left\| \boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}_{\boldsymbol{q}} \right\|^2$$

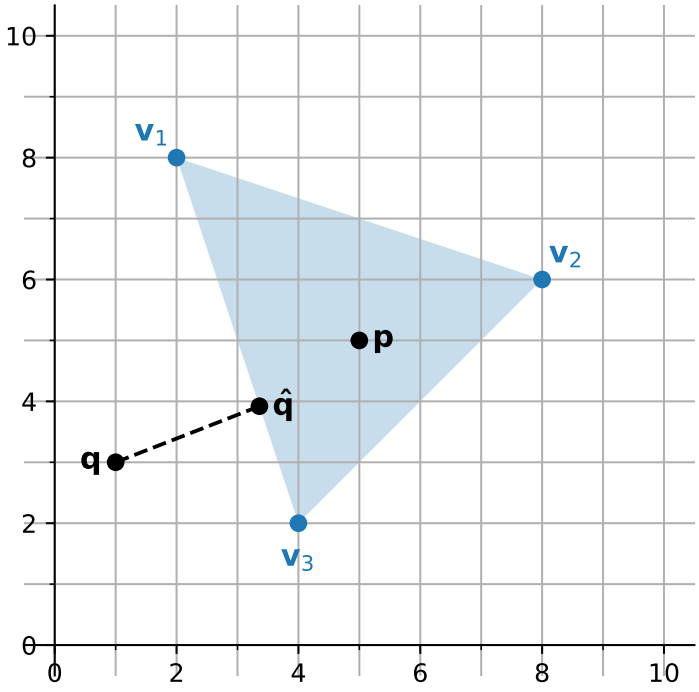
and have a look at your result. Does it agree with the required convexity constraints? Again, compute $\boldsymbol{V}\boldsymbol{w}_\star$ but now compare it to $\boldsymbol{q}$. What do you observe? What is going on here?

task 1.5.2 [8 points]

The following figure extends the one above in that it also shows the point

$$\hat{\boldsymbol{q}} = \underset{\boldsymbol{x} \in \Delta(\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3)}{\operatorname{argmin}} \left\| \boldsymbol{q} - \boldsymbol{x} \right\|^2 . \tag{16}$$

which is the closest point to $\boldsymbol{q}$ in $\Delta\big(\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3\big)$.



Implement code that solves the optimization problem in (16) and provide your result. Furthermore, determine the barycentric coordinates of $\hat{\boldsymbol{q}}$ and provide your results.

task 1.6

submission of presentation and code

Prepare a set of slides about your solutions and results for tasks 1.2, 1.3, 1.4, and 1.5.

These slides should help you to give a scientific presentation of your work, i.e. to give a short talk in front of your fellow students and instructors and to answer any questions they may have.

W.r.t. to formalities, please make sure that

- your presentation contains a title slide which lists the names and matriculation numbers of everybody in your team who contributed to the solutions.

W.r.t. content, please make sure that

- your presentation contains about 12 to 15 content slides but not more
- your presentation is concise (not at all overly verbose!!!) and clearly structured; **your goal must be to focus on the essence of a topic**
- your presentation answers questions such as
  - "what was the task / problem we considered?"
  - "what kind of difficulties (if any) did we encounter?"
  - "how did we solve them?"
  - "what were our results?"
  - "what did we learn?"

Save / export your slides as a PDF file and upload it to eCampus.

Furthermore, please name all your code files in a manner that indicates which task they solve (e.g. `task-1-3.py`) and put them in an archive or a ZIP file.

Upload this archive / ZIP file to eCampus.