EX.4.1.8.a, Sauer3

Find the best line through each set of data points, and find the RMSE

$$(0,0), \quad (1,3), \quad (2,3), \quad (5,6).$$

EX.4.1.8.a, Sauer3, solution, Langou

Colab: `https://colab.research.google.com/drive/1-t_9FiXuS5PlzpZeB3vVY6IxLS_6hf4d`

Setting

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 5 \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} 0 \\ 3 \\ 3 \\ 6 \end{bmatrix},$$

we form the linear least squares problem

$$\min_{x\in\mathbb{R}^2} \| \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 5 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} - \begin{bmatrix} 0 \\ 3 \\ 3 \\ 6 \end{bmatrix} \|_2.$$

First we form

$$A^T A = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 5 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 5 \end{bmatrix} = \begin{bmatrix} 4 & 8 \\ 8 & 30 \end{bmatrix}.$$

and

$$A^T b = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 5 \end{bmatrix} \begin{bmatrix} 0 \\ 3 \\ 3 \\ 6 \end{bmatrix} = \begin{bmatrix} 12 \\ 39 \end{bmatrix}.$$

Now we solve $(A^T A)x = (A^T b)$. We get the least squares solution as

$$\begin{bmatrix} 4 & 8 \\ 8 & 30 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 12 \\ 39 \end{bmatrix} \quad \Longrightarrow \quad \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \frac{1}{56} \begin{bmatrix} 30 & -8 \\ -8 & 4 \end{bmatrix} \begin{bmatrix} 12 \\ 39 \end{bmatrix} = \frac{1}{56} \begin{bmatrix} 48 \\ 60 \end{bmatrix} = \frac{3}{14} \begin{bmatrix} 4 \\ 5 \end{bmatrix}$$

We find that the best-fit line in the least squares sense that fits our data point is

$$y = \frac{6}{7} + \frac{15}{14}x.$$

We can compute the residual

$$r = b - Ax = \begin{bmatrix} 0 \\ 3 \\ 3 \\ 6 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 5 \end{bmatrix} \frac{3}{14} \begin{bmatrix} 4 \\ 5 \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \\ 3 \\ 6 \end{bmatrix} - \frac{3}{14} \begin{bmatrix} 4 \\ 9 \\ 14 \\ 29 \end{bmatrix} = \frac{3}{14} (\begin{bmatrix} 0 \\ 14 \\ 14 \\ 28 \end{bmatrix} - \begin{bmatrix} 4 \\ 9 \\ 14 \\ 29 \end{bmatrix}) = \frac{3}{14} \begin{bmatrix} -4 \\ 5 \\ 0 \\ -1 \end{bmatrix})$$

The 2-norm error is

$$\|r\|_2 = \frac{3}{14}\sqrt{(-4)^2 + (5)^2 + (0)^2 + (-1)^2} = \frac{3}{14}\sqrt{42}.$$

The root mean squared error (RMSE) is

$$\text{RMSE} = \frac{\|r\|_2}{\sqrt{m}} = \frac{3}{28}\sqrt{42} \approx 0.694.$$

What is below is not needed.

Check:

$$A^T r = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 5 \end{bmatrix} \frac{3}{14} \begin{bmatrix} -4 \\ 5 \\ 0 \\ -1 \end{bmatrix}) = \frac{3}{14} \begin{bmatrix} (1)(-4) + (1)(5) + (1)(0) + (1)(-1) \\ (0)(-4) + (1)(5) + (2)(0) + (5)(-1) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \qquad \checkmark$$

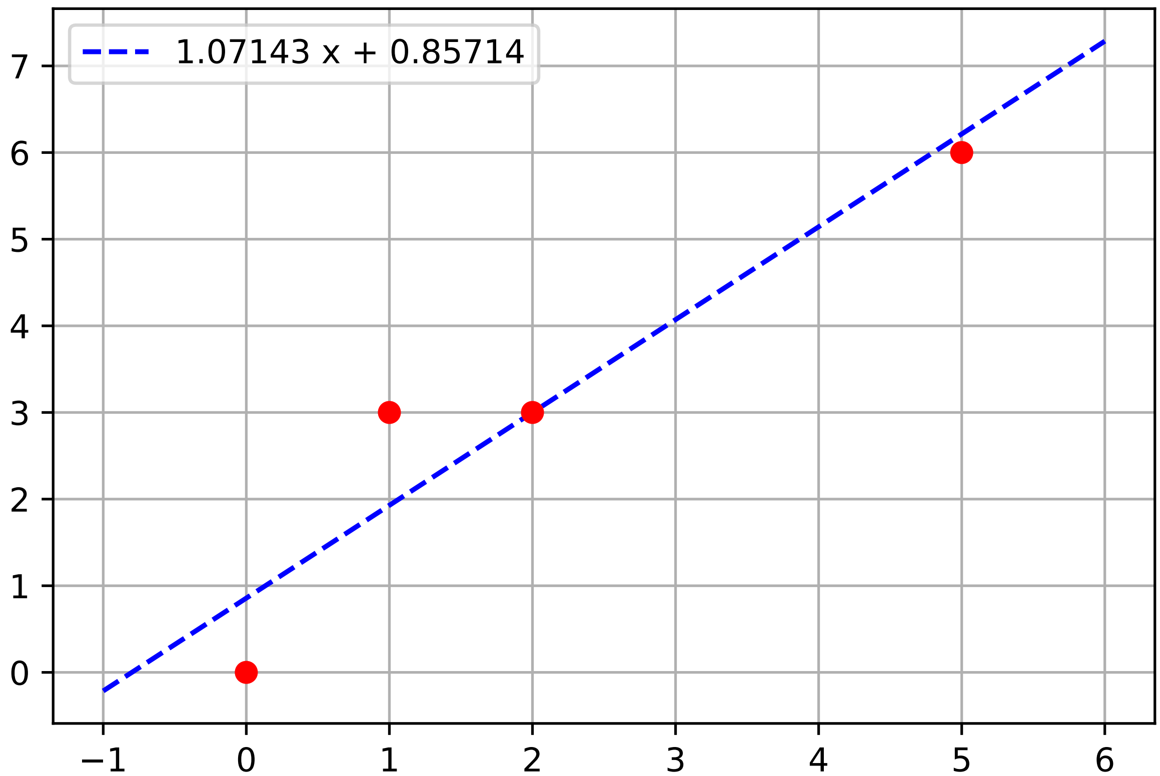
What is below is not needed.

Python helper notebook:

```
import numpy as np
from math import sqrt
import matplotlib.pyplot as plt

data = np.array([
        [0.,0.],
        [1.,3.],
        [2.,3.],
        [5.,6.] ])

xx = data[:,0]
yy = data[:,1]

A = np.array([ np.ones( xx.shape ), xx ]).T
b = np.array([ yy ]).T
print("A =\n",A)
print("b =\n",b)

# compute x either using np.linalg.lstsq or normal equation methods
# x = np.linalg.lstsq(A,b,rcond=None)[0]
x = np.linalg.solve( A.T@A, A.T@b )

print("x =\n",x)
print("r =\n",b-A@x)
print("|| b - Ax ||_2 = ", f"{np.linalg.norm( A@x - b, 2 ):.4f}")
print("|| A^T ( b - Ax ) ||_oo =",
      f"{np.linalg.norm( A.T@( A@x - b), np.infty ):.1e}" )

# plot
xxx = np.linspace( -1., 6., 10)
yyy = x[0] + x[1] * xxx
label_ = f'{x[1,0]:7.5f}'+' x + '+f'{x[0,0]:7.5f}'
plt.plot(xxx, yyy, '--b',label=label_)
```

```
plt.plot( xx, yy, 'ro')
plt.legend()
plt.grid()
plt.show()
```

```
A =
 [[1. 0.]
 [1. 1.]
 [1. 2.]
 [1. 5.]]
b =
 [[0.]
 [3.]
 [3.]
 [6.]]
x =
 [[0.85714286]
 [1.07142857]]
[ Ax, b ]=
 [[0.85714286 0.        ]
 [1.92857143 3.        ]
 [3.         3.        ]
 [6.21428571 6.        ]]
r =
 [[-0.85714286]
 [ 1.07142857]
 [ 0.        ]
 [-0.21428571]]
|| b - Ax ||_2 =  1.3887
RMSE =  0.6944
|| A^T ( b - Ax ) ||_oo = 3.8e-15
```


1.07143 x + 0.85714
7
6
5
4
3
2
1
0
−1
0
1
2
3
4
5
6