

Assignment 2 - Numerical Linear Algebra

Prof.: Bernardo Freitas Paulo da Costa

TA: Beatriz Lúcia Teixeira de Souza

Student: Arthur Rabello Oliveira

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1. Problem 1: Traditional Least Squares (a - f)

1.1. Linear Regression (a)

We have a set of equally spaced points $S := \{t_i = \frac{i}{m}\}, i = 0, 1, \dots, m$, we will find the best line $f(t) = \alpha + \beta t$ that approximates the points $(t_i, b_i) \in \mathbb{R}^2$

The system of equations to be solved is to be given as a function of t_i, b_i, m .

Solution:

Approximating 2 points in \mathbb{R}^2 by a line is trivial, now approximating more than 2 points is a task that requires linear algebra. To see this, we will analyze the following example to build intuition for the general case:

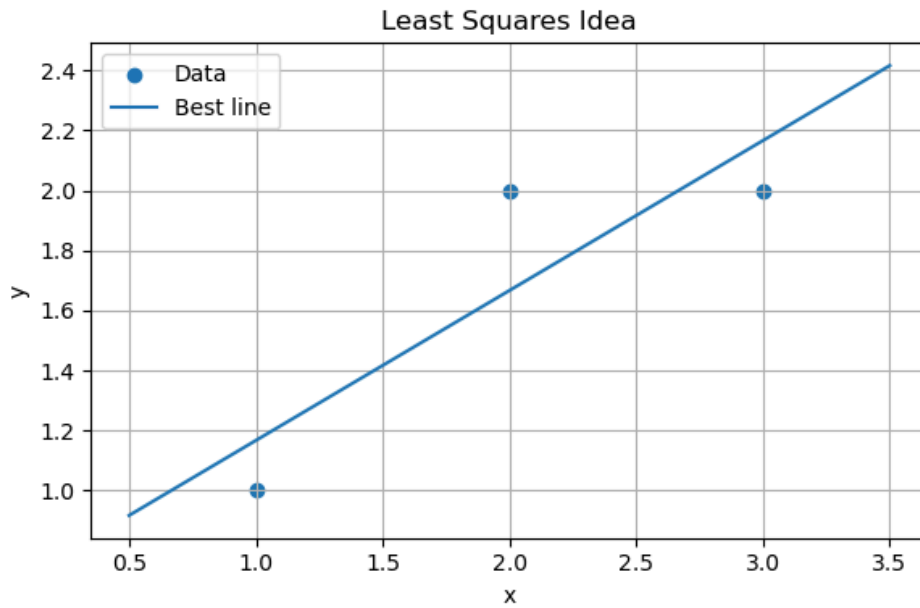


Figure 1: A glimpse into what we want to see

Given the points $(1, 1), (2, 2), (3, 2) \in \mathbb{R}^2$, we would like a line $f(t) = y(t) = \alpha + \beta t$ that best approximates these 3 points, in other words, since we know that the line does not pass through all of the 3 points, we would like to find the *closest* line to the line that would pass through the 3 points, so the system:

$$\begin{aligned} f(1) &= \alpha + \beta = 1 \\ f(2) &= \alpha + 2\beta = 2 \\ f(3) &= \alpha + 3\beta = 2 \end{aligned} \tag{1}$$

Clearly has no solution, (the line does not cross the 3 points), but it has a *closest solution*, which we can find through **projections**, the system is:

$$\underbrace{\begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix}}_A \cdot \underbrace{\begin{pmatrix} \alpha \\ \beta \end{pmatrix}}_x = \underbrace{\begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix}}_b \tag{2}$$

Let $x^* \neq x$ be a solution to the system, we want to **minimize** the error produced by approximating the points through a line, so if the **error** is $e = Ax - b$, we want the smaller error *square* possible (that is why least squares). We square the error to avoid and detect outliers, so:

$$e_1^2 + e_2^2 + e_3^2 \quad 3$$

Is what we want to minimize, where e_i is the error (distance) from the i th point to the line:



Figure 2: The errors (distances)

In this case, we will project this system into the column space of the matrix A , giving us the closest solution, and the least squares solutions is when \hat{x} minimizes $\|Ax - b\|^2$, this occurs when the residual $e = Ax - b$ is orthogonal to $C(A)$, since $N(A^T) \perp C(A)$ and the dimensions sum up the left dimension of the matrix, so:

$$\begin{aligned} A^T A \hat{x} &= A^T b \\ &= \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix} \cdot \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \cdot \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 3 & 6 \\ 6 & 14 \end{pmatrix} \cdot \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \\ &= \begin{pmatrix} 3 & 6 \\ 6 & 14 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 5 \\ 11 \end{pmatrix} \end{aligned} \quad 4$$

So the system to find $\hat{x} = \begin{pmatrix} \hat{\alpha} \\ \hat{\beta} \end{pmatrix}$ becomes:

$$\begin{aligned} 3\alpha + 5\beta &= 5 \\ 6\alpha + 14\beta &= 11 \end{aligned} \quad 5$$

Notice that with the *errors* e_i^2 as:

$$\begin{aligned} e_1^2 &= (\alpha + \beta - 1)^2 \\ e_2^2 &= (\alpha + 2\beta - 2)^2 \\ e_3^2 &= (\alpha + 3\beta - 2)^2 \end{aligned} \quad 6$$

The system in eq. (5) is *precisely* what is obtained after using partial derivatives to minimize the erros sum as a function of (α, β) :

$$\begin{aligned} f(\alpha, \beta) &= (\alpha + \beta - 1)^2 + (\alpha + 2\beta - 2)^2 + (\alpha + 3\beta - 2)^2 \\ &= 3\alpha^2 + 14\beta^2 + 12\alpha\beta - 10\alpha - 22\beta + 9, \\ \frac{\partial f}{\partial \alpha} = \frac{\partial f}{\partial \beta} = 0 &\Leftrightarrow 6\alpha + 12\beta - 10 = 28\beta + 12\alpha - 22 = 0 \Leftrightarrow \begin{cases} 3\alpha + 6\beta = 5 \\ 6\alpha + 14\beta = 11 \end{cases} \end{aligned} \quad 7$$

This new system has a solution in $\hat{\alpha} = \frac{2}{3}, \hat{\beta} = \frac{1}{2}$, so the equation of the optimal line, obtained through *linear regression* (or least squares) is:

$$y(t) = \frac{2}{3} + \frac{1}{2}t. \quad 8$$

If we have $n > 3$ points to approximate through a line, the reasoning is analogous:

With $S := \{t_i = \frac{i}{m}, i = 0, 1, \dots, m\}$, we will find the best *line* $f(t) = \alpha + \beta t$ that approximates the points $(t_i, b_i) \in \mathbb{R}^2$

The system of equations to be solved be given as a function of t_i, b_i, m .

We want to find the extended system as we did in eq. (7), so our line is:

$$f(t) = \alpha + \beta t \quad 9$$

That best approximates the points $(0, b_0), (\frac{1}{m}, b_1), \dots, (1, b_m)$. The system is:

$$\begin{aligned} f(0) &= b_0 = \alpha, \\ f\left(\frac{1}{m}\right) &= b_1 = \alpha + \frac{\beta}{m}, \\ f\left(\frac{2}{m}\right) &= b_2 = \alpha + \frac{2}{m}\beta \\ &\vdots \\ f(1) &= b_m = \alpha + \beta \end{aligned} \quad 10$$

And the $Ax = b$ matrices alternative:

$$\underbrace{\begin{pmatrix} 1 & 0 \\ 1 & \frac{1}{m} \\ \vdots & \vdots \\ 1 & 1 \end{pmatrix}}_A \cdot \underbrace{\begin{pmatrix} \alpha \\ \beta \end{pmatrix}}_x = \underbrace{\begin{pmatrix} b_0 \\ \vdots \\ b_m \end{pmatrix}}_b \quad 11$$

Projecting into $C(A)$, we have:

$$\begin{aligned} A^T A x &= A^T b \\ &= \begin{pmatrix} 1 & 1 & \dots & 1 \\ 0 & \frac{1}{m} & \dots & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 1 & \frac{1}{m} \\ \vdots & \vdots \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} m+1 & \frac{m+1}{2} \\ \frac{m+1}{2} & \frac{(m+1)(2m+2)}{6m} \end{pmatrix} \cdot \begin{pmatrix} \hat{\alpha} \\ \hat{\beta} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 1 & \dots & 1 \\ 0 & \frac{1}{m} & \dots & 1 \end{pmatrix} \cdot \begin{pmatrix} b_0 \\ \vdots \\ b_m \end{pmatrix} = \begin{pmatrix} b_0 + b_1 + \dots + b_m \\ \frac{1}{m}[b_1 + 2b_2 + \dots + (m-1)b_m] \end{pmatrix} \end{aligned} \quad 12$$

So the new system to be solved is:

$$\begin{pmatrix} m+1 & \frac{m+1}{2} \\ \frac{m+1}{2} & \frac{(m+1)(2m+2)}{6m} \end{pmatrix} \cdot \begin{pmatrix} \hat{\alpha} \\ \hat{\beta} \end{pmatrix} = \begin{pmatrix} b_1 + b_2 + \dots + b_m \\ \frac{1}{m}[b_2 + 2b_3 + \dots + (m-1)b_m] \end{pmatrix} \quad 13$$

Or:

$$\begin{pmatrix} m+1 & \sum_{i=1}^m t_i \\ \sum_{i=1}^m t_i & \sum_{i=1}^m t_i^2 \end{pmatrix} \cdot \begin{pmatrix} \hat{\alpha} \\ \hat{\beta} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^m b_i \\ \sum_{i=1}^m \frac{i}{m} \cdot b_i \end{pmatrix} \quad 14$$

1.2. The Conditioning number of a matrix (b)

1.2.1. Conditioning Number of matrices

1.2.2. Application

1.3. More Regression: A Polynomial Perspective (c)

1.4. Finding the matrix A through Python (d)

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