GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

Mathematics and Computer Science (B.MES.108)
Summer Semester, 2020
Part 1: Linear Algebra for Non-Mathematicians

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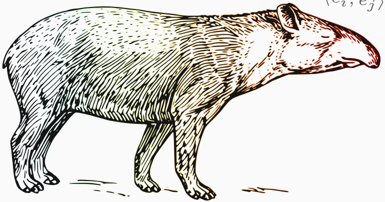
$(AB)^{\top} = B^{\top} A^{\top}$ $\quad \mathbb{R}^n \xrightarrow{T} \mathbb{R}^m$

$\vec{v} = \sum_{i=1}^{n} \alpha_i \hat{e}_i$ $\quad A = Q\Lambda Q^{-1}$

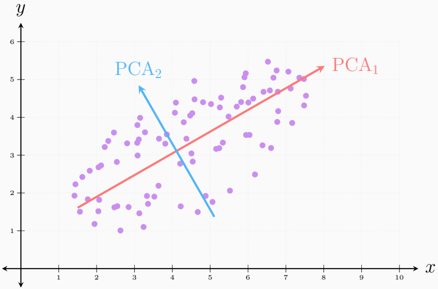
$\mathrm{Rot}(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$ $\quad A\vec{v} = \lambda\vec{v}$

$T(\alpha\vec{u} + \beta\vec{v}) = \alpha T(\vec{u}) + \beta T(\vec{v})$

$\langle \hat{e}_i, \hat{e}_j \rangle = \delta_{ij}$

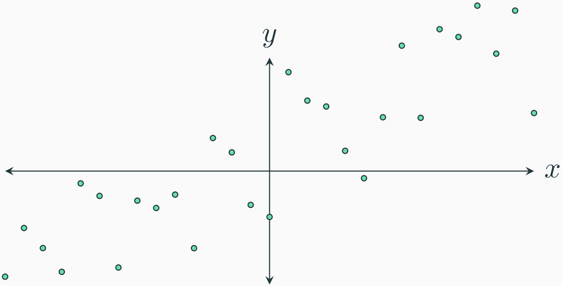


Chapter 7: Some Real-World Uses of Linear Algebra



Least Squares Approximation

What is the best linear approximation to a set of measurements?



Least Squares Approximation

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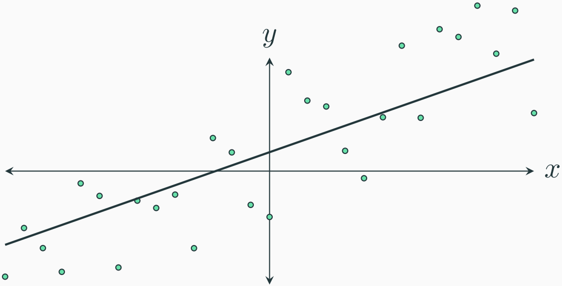

Least Squares Approximation

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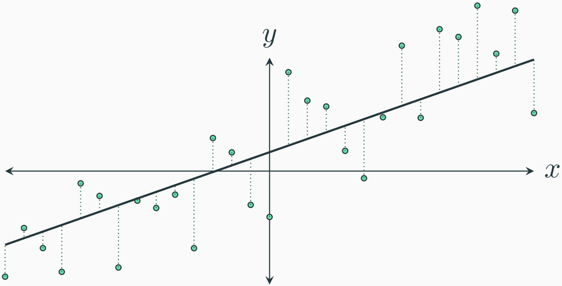


A good approximation is the line $f(x) = ax + b$ for which the sum of the distances from the line to each point (x_i, y_i) is minimal, i.e.

$$S = \min \left(\sum_{i=1}^{n} \left[f\left(x_i\right) - y_i \right] \right).$$

Least Squares Approximation

We can collect all the y values of our measurement points to a vector:

$$\vec{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix},$$

and similarly collect all the $y = f(x)$ values of the line:

$$\vec{f} = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \end{pmatrix}.$$

Least Squares Approximation

The sum $s = \sum_{i=1}^{n} \left[f\left(x_i\right) - y_i\right]$ then becomes:

$$s = \sum_{i=1}^{n} \left[f\left(x_i\right) - y_i\right]$$
$$= \sum_{i=1}^{n} \left[\vec{f_i} - \vec{y_i}\right].$$

However, s is a bit problematic, as some elements $\vec{f_i} - \vec{y_i}$ can be negative. Instead, we can minimize the following expression:

$$s^* = \sum_{i=1}^{n} \left[\vec{f_i} - \vec{y_i}\right]^2.$$

Least Squares Approximation

...and the expression

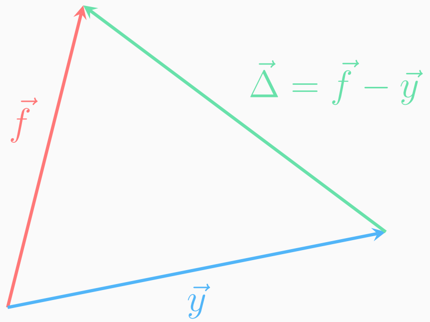
$$s^* = \sum_{i=1}^{n} \left[\vec{f_i} - \vec{y_i}\right]^2$$

is exactly the square norm of the vector

$$\vec{\Delta} = \begin{pmatrix} f_1 - y_1 \\ f_2 - y_2 \\ \vdots \\ f_n - y_n \end{pmatrix} = \vec{f} - \vec{y}.$$

Least Squares Approximation

Drawing the a 2-dimentional scheme of the vectors $\vec{v}, \vec{f}$ and their difference $\vec{\Delta} = \vec{f} - \vec{v}$:



Least Squares Approximation

The norm of the vector $\vec{\Delta} = \vec{f} - \vec{y}$ is minimal when $\vec{f} \perp \vec{\Delta}$, i.e. when

$$\vec{f} \cdot \vec{\Delta} = \vec{f} \cdot \left(\vec{f} - \vec{y} \right) = 0.$$

Let's find what condition on $\vec{f}$ yields this.

Least Squares Approximation

First, we note that the vector $\vec{f}$ can be written as a matrix-vector product:

$$\vec{f} = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \end{pmatrix} = \begin{pmatrix} ax_1 + b \\ ax_2 + b \\ \vdots \\ ax_n + b \end{pmatrix} = \underbrace{\begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \\ x_n & 1 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} a \\ b \end{pmatrix}}_{v}.$$

Thus, the condition $\vec{f} \cdot \left(\vec{f} - \vec{y}\right) = 0$ becomes

$$A\vec{v} \cdot (A\vec{v} - \vec{y}) = 0.$$

Least Squares Approximation

Some algebra:

$$A\vec{v} \cdot (A\vec{v} - \vec{y}) = 0.$$

Least Squares Approximation

Some algebra:

$$A\vec{v} \cdot A\vec{v} - A\vec{v} \cdot \vec{y} = 0.$$

Least Squares Approximation

Some algebra:

$$A\vec{v} \cdot A\vec{v} = A\vec{v} \cdot \vec{y}.$$

Least Squares Approximation

Some algebra:

$$A\vec{v} \cdot A\vec{v} = A\vec{v} \cdot \vec{y}.$$

Since $A\vec{v}$ is a vector, it can be dotted with either itself or $\vec{y}$. However, we can consider $A\vec{v}$ as an $n \times 1$ matrix, and to keep the product defined we transpose it, i.e.

$$(A\vec{v})^{\top} \cdot A\vec{v} = (A\vec{v})^{\top} \cdot \vec{y}.$$

This doesn't change the truthness of the equation.

Least Squares Approximation

Expanding the transposed product $(A\vec{v})^\top$ yields

$$\vec{v}^\top A^\top A\vec{v} = \vec{v}^\top A^\top \vec{y},$$

where $\vec{v}^\top$ is a row vector.

We can remove $\vec{v}^\top$ from both sides, leaving us with

$$A^\top A\vec{v} = A^\top \vec{y}.$$

This linear system is surprisingly easy to solve!

Least Squares Approximation

Example

Let's look at 6 points:

$$p_1 = (-2, -7.3)$$
$$p_2 = (-1, -3.9)$$
$$p_3 = (0, -1.2)$$
$$p_4 = (1, 2.4)$$
$$p_5 = (2, 4.7)$$
$$p_6 = (3, 7.7)$$

Example

The linear system we need to solve is thus

$$\begin{pmatrix} -2 & -1 & 0 & 1 & 2 & 3 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} -2 & 1 \\ -1 & 1 \\ 0 & 1 \\ 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} -2 & -1 & 0 & 1 & 2 & 3 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} -7.3 \\ -3.9 \\ -1.2 \\ 2.4 \\ 4.7 \\ 7.7 \end{pmatrix}.$$

Multiplying both matrix-matrix products yields

$$\begin{pmatrix} 19 & 3 \\ 3 & 6 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 53.4 & 2.4 \end{pmatrix},$$

which when solved for a and b yields

$$a = 2.98 \quad b = -1.09.$$

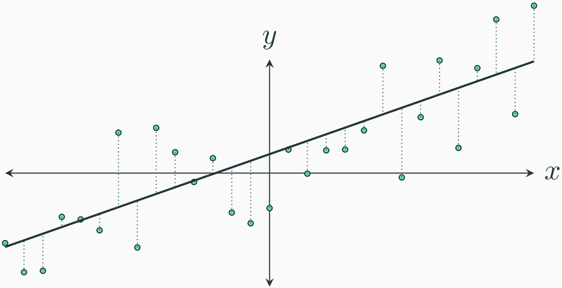
Least Squares Approximation

How can we quantify the "goodness" of fit between the proposed approximation and out data points?

Least Squares Approximation

We can first look at the average difference between y_i and the linear approximation (the **variance** in the y-values in respect to the line):

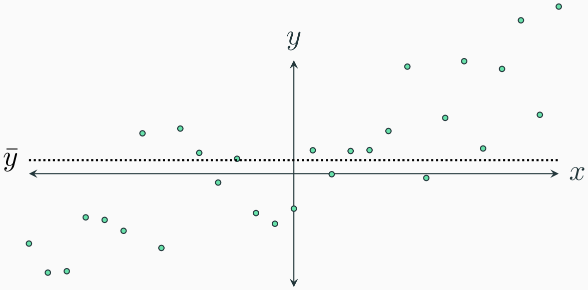
$$\sigma_{\text{line}} = \frac{1}{n} \sum_{i=1}^{n} \left[f\left(x_i\right) - y_i \right]^2 .e$$



Least Squares Approximation

Then we look at the average y value of our data points:

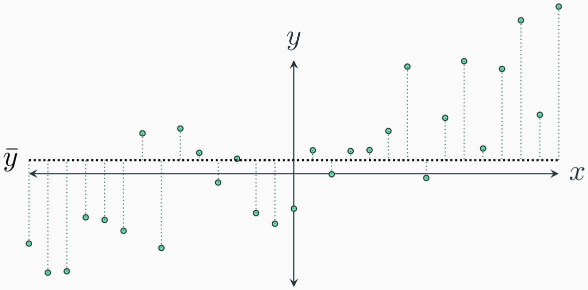
$$\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i.e$$



Least Squares Approximation

We can calculate the total distance of out data points to $\bar{y}$:

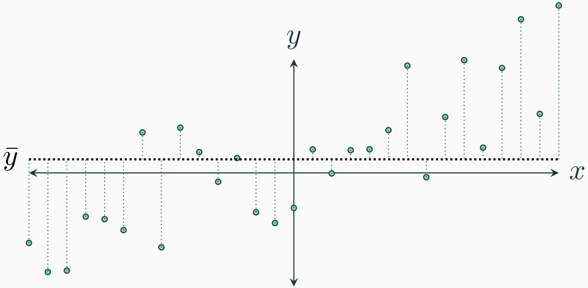
$$\mathsf{SE}_{\bar{y}} = (y_1 - \bar{y})^2 + (y_2 - \bar{y})^2 + \cdots + (y_n - \bar{y})^2 = \sum_{i=1}^{n} (y_i - \bar{y})^2 .e$$



Least Squares Approximation

The average of $\mathsf{SE}_{\bar{y}}$ is the variance in the y-values:

$$\sigma_y = \frac{1}{n}\mathsf{SE}_{\bar{y}} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2\,.e$$



Least Squares Approximation

The ratio of the two variances

$$\rho = \frac{\sigma_{\text{line}}}{\sigma_{\bar{y}}}$$

is a measurement of what percentage of the total variation is **NOT** described by the linear approximaion. It is in the range

$$0 \leq \rho \leq 1.$$

Thus,

$$r^2 \equiv 1 - \rho = 1 - \frac{\sigma_{\text{line}}}{\sigma_{\bar{y}}}$$

describes how much of the total variation is described by the linear approximation.

Least Squares Approximation

An r^2 close to 1 means that ρ is close to 0, i.e. the variation of y_i from the line, σ_{line}, is small compared to the total variance of the points.

Least Squares Approximation

Example

The average y value of the points in the previous example is

$$\bar{y} = \frac{1}{6}\left(-7.3 - 3.9 - 1.2 + 2.4 + 4.7 + 7.7\right) = \frac{2.4}{6} = 0.4.$$

Their total variance is thus

$$\begin{aligned}\sigma_{\bar{y}} &= \frac{1}{6}\Big[(-7.3-0.4)^2 + (-3.9-0.4)^2 + (-1.2-0.4)^2 \\ &\quad + (2.4-0.4)^2 + (4.7-0.4)^2 + (7.7-0.4)^2\Big] \\ &= \frac{1}{6}\left[59.29 + 18.49 + 2.56 + 4 + 18.49 + 53.29\right] \\ &= 26.02.\end{aligned}$$

Least Squares Approximation

Example

The linear approximation was calculated as $f(x) = 2.98x - 1.09$, and so the variance to the linear approximation is

$$\begin{aligned}
\sigma_{\mathsf{line}} &= \frac{1}{6}\Big[(-7.05+7.3)^2 + (-4.07+3.9)^2 + (-1.09+1.2)^2 \\
&\quad +(1.89-2.4)^2 + (4.87-4.7)^2 + (7.85-7.7)^2\Big] \\
&= \frac{1}{6}\left[0.06+0.03+0.01+0.26+0.03+0.02\right] \\
&= 0.0692.
\end{aligned}$$

Example

Thus,

$$r^2 = 1 - \frac{\sigma_{\text{line}}}{\sigma_{\bar{y}}} = 1 - \frac{0.0692}{26.02} = 1 - 0.0027 = 0.9973,$$

which means that the linear approximation given by the least squares method for this set of points is an exceptionally good approximation.