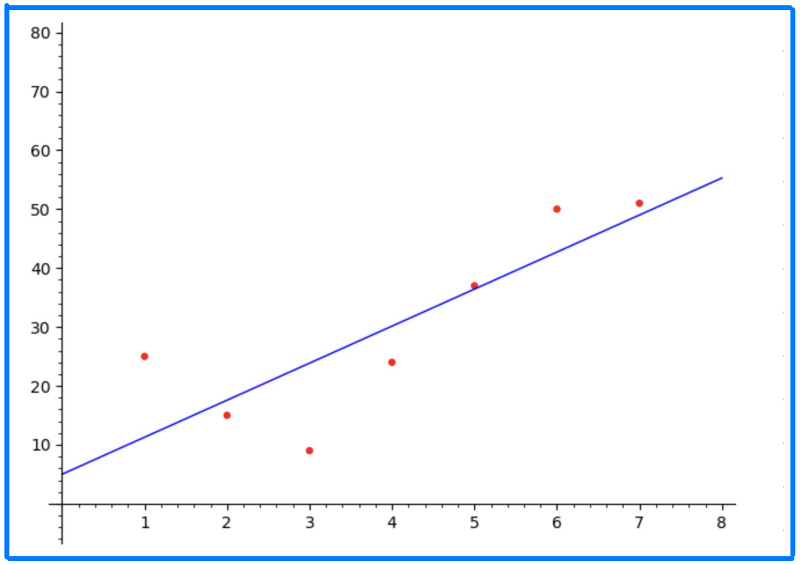
Proseminar on computer-assisted mathematics

Session 4 - Least squares approximation



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What we want to be able to do:

- Perform data analysis using linear regression.
- Starting from a data set, find a good approximation model and use that model to:
    1. Describe and analyse the data.
    2. Make some predictions for the future.

The concrete problem

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show(data)
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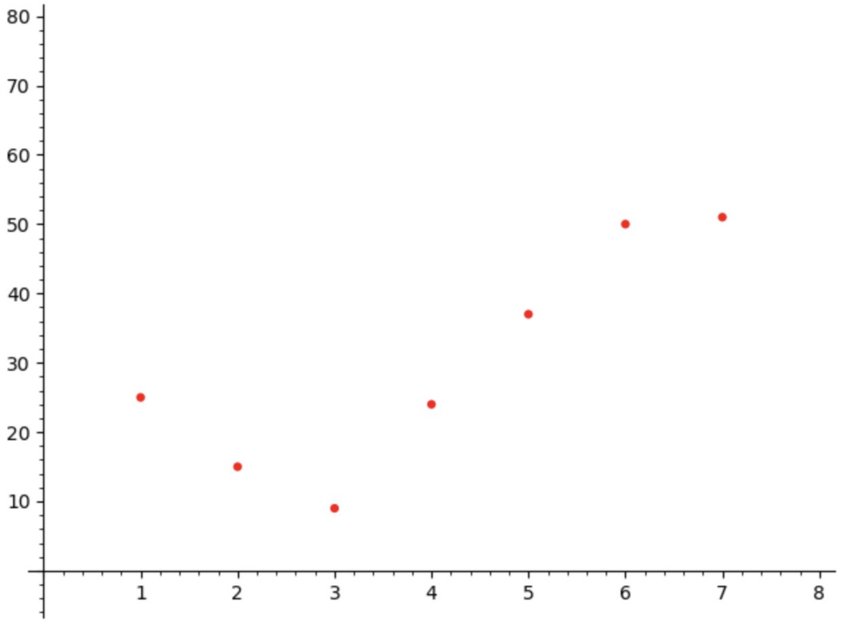
$[(1,25),(2,15),(3,9),(4,24),(5,37),(6,50),(7,51)]$



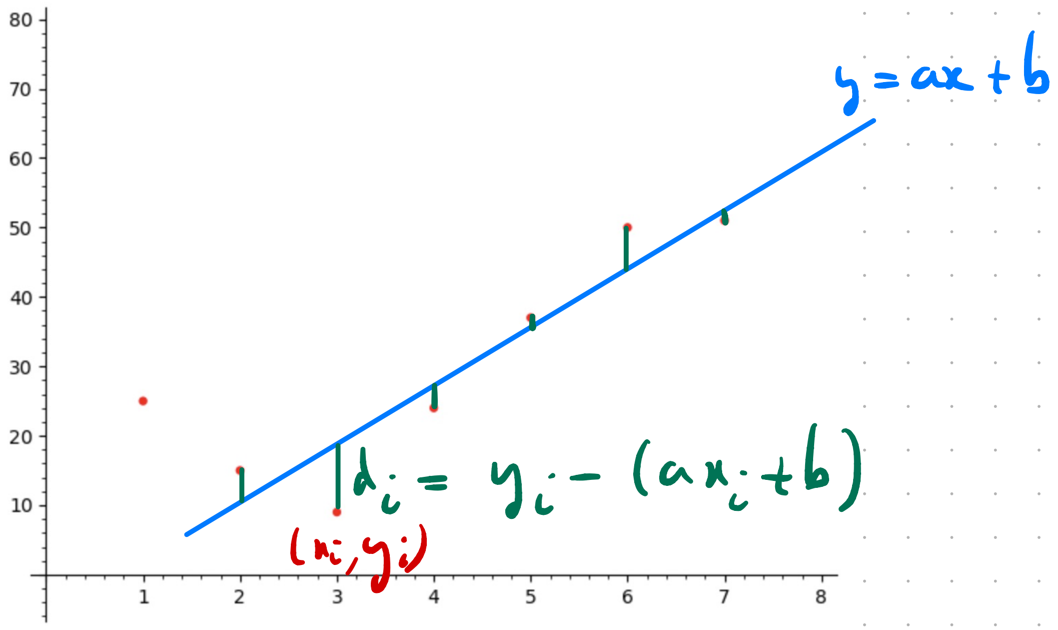
We start from a data set.

We look at the associated scatter plot in the plane.

We try to approximate the scatter plot by a line or a parabola, or whatever model we consider relevant.

The mathematical formulation

Choose for instance $y = ax + b$ as a model: this means that we try to approximate the scatter plot by an affine line.



We want to minimise the quantity

$$d_1^2 + d_2^2 + \dots + d_n^2 .$$

"Least squares approximation"

We solve the problem using linear algebra:

$$Y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \qquad A = \begin{pmatrix} x_1 & 1 \\ \vdots & \\ x_n & 1 \end{pmatrix} \qquad X = \begin{pmatrix} a \\ b \end{pmatrix}$$

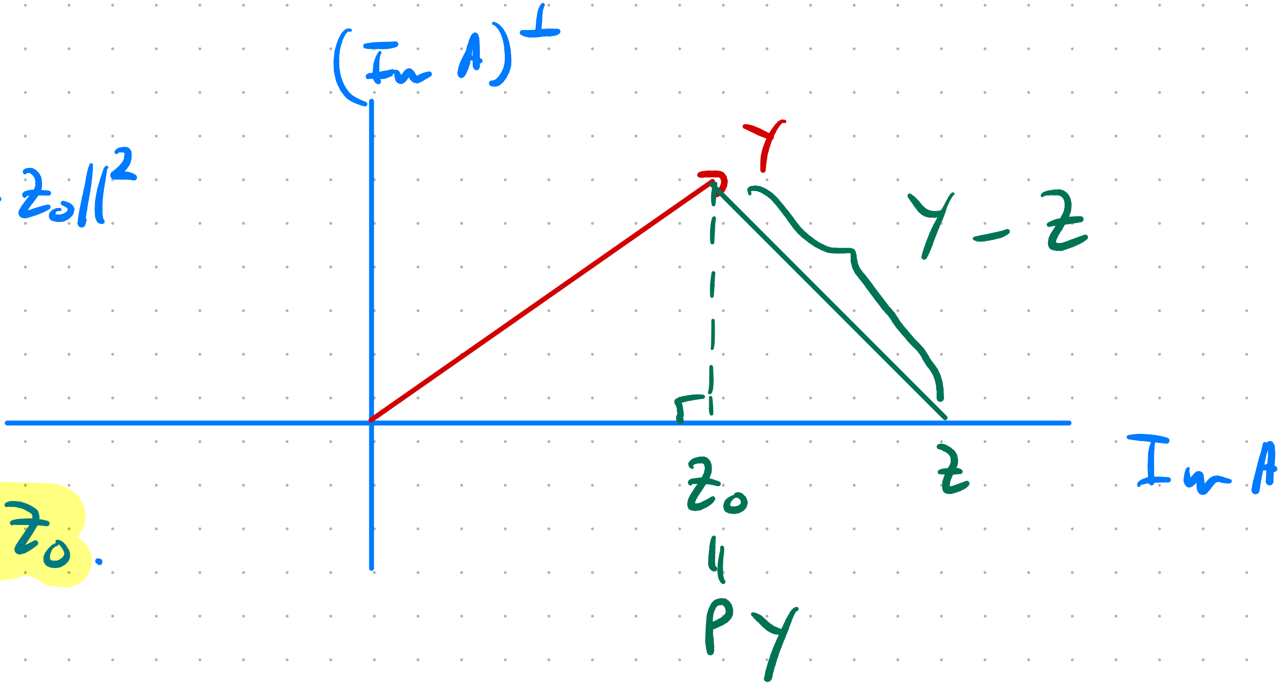
$$\min_{(a,b)\in\mathbb{R}^2} \overbrace{\|Y - AX\|^2}^{= d_1^2 + \dots + d_n^2}$$

Pythagorean theorem!

$$\|Y - Z\|^2 = \|Y - Z_0\|^2 + \|Z - Z_0\|^2$$

$$\geq \|Y - Z_0\|^2$$

with equality if and only if $Z = Z_0$.



Explicit formulas

Projection matrix:

If A has full rank, then $P = A\,(A^t A)^{-1} A^t$ is the projection matrix.

Solution of the least squares problem:

If A has full rank, then $\| Y - AX \|^2$ is minimal iff $X = (A^t A)^{-1} A^t Y$

(so indeed $AX = PY$).

A proof of the formula for the projection matrix

$$z_0 = P_{\mathrm{Im}\,A}(Y) \quad \text{iff} \quad \begin{cases} z_0 \in \mathrm{Im}\,A \\ (Y - z_0) \in (\underbrace{\mathrm{Im}\,A}_{})^{\perp} \end{cases}$$

$$\text{iff} \quad \begin{cases} z_0 = AX \\ (Y - AX) \in \mathrm{Ker}\,A^t \end{cases}$$

exercise! (they are equal subspaces)

i.e. $A^t(Y - AX) = 0$ exercise! invertible if A has full rank

i.e. $A^t Y = A^t(AX) = \overbrace{(A^t A)}^{} X$

i.e. $X = (A^t A)^{-1} A^t Y$

i.e. $z_0 = AX = A(A^t A)^{-1} A^t Y.$