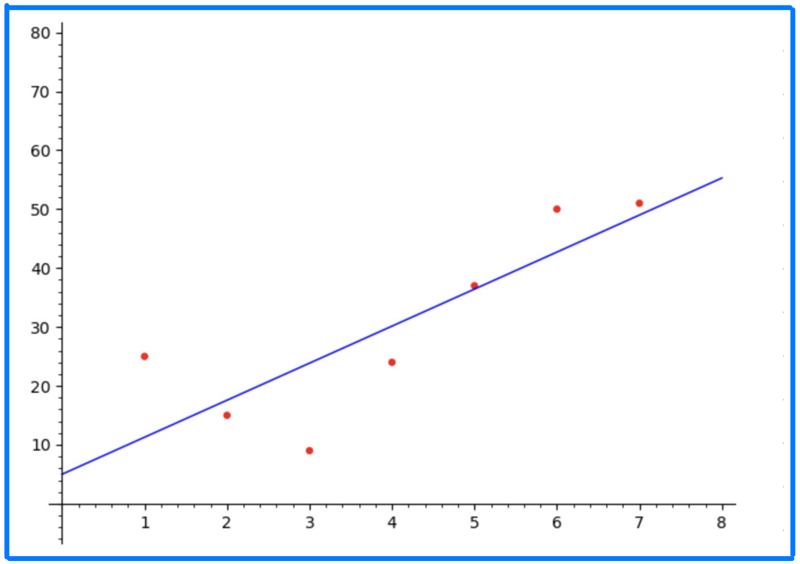
Proseminar on computer-assisted mathematics

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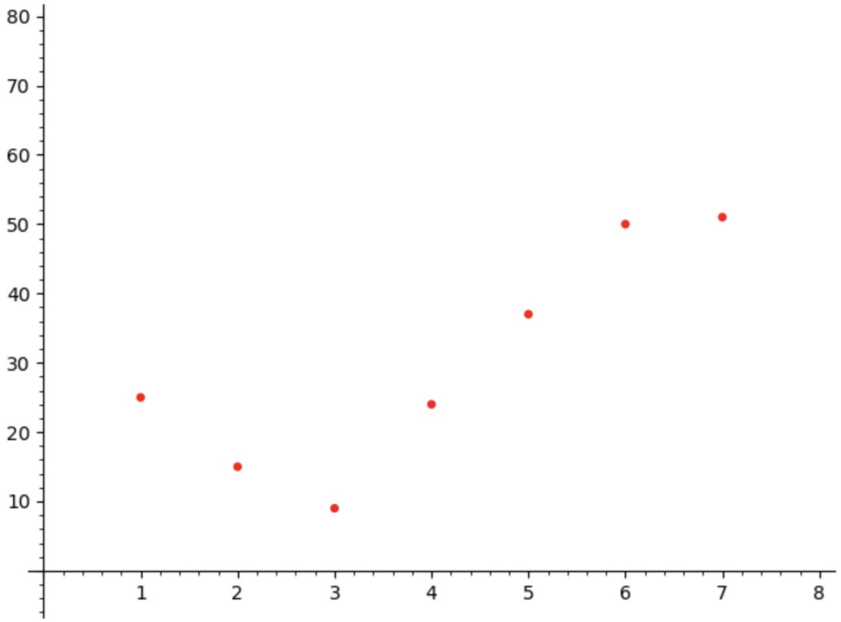
$[(1,25),(2,15),(3,9),(4,24),(5,37),(6,50),(7,51)]$



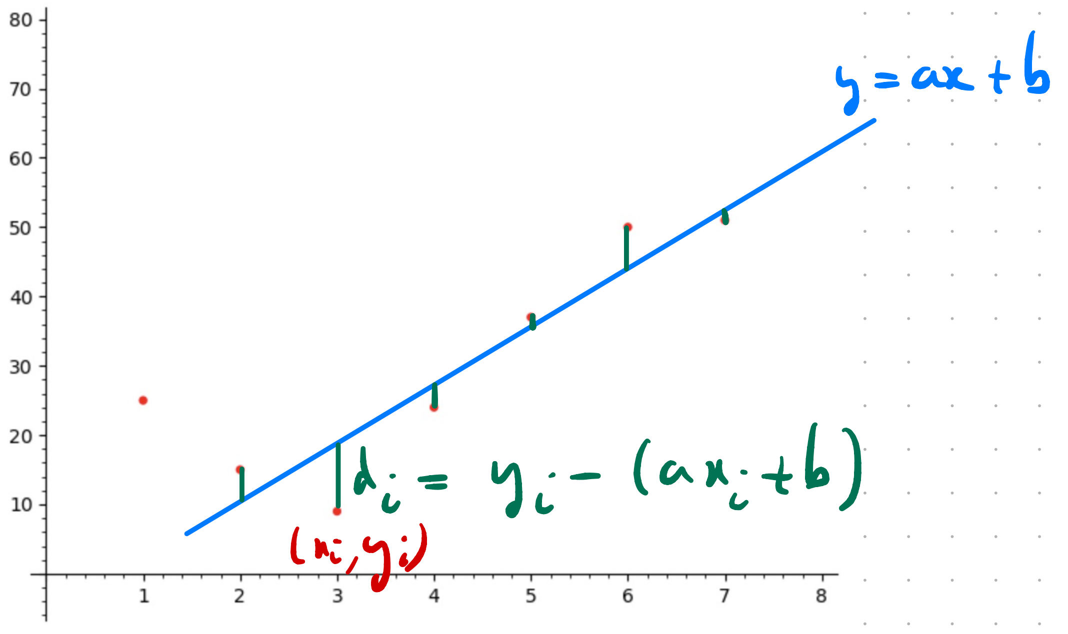
We start from a data set.

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 need 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.

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

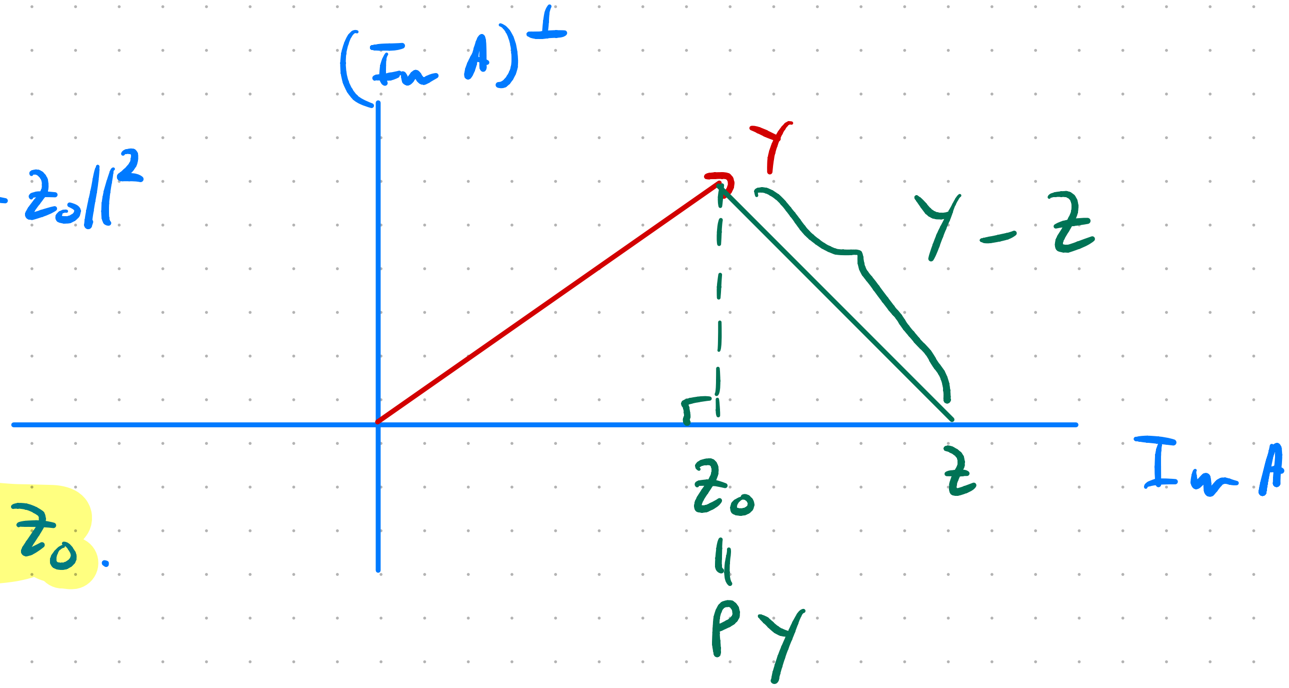
$$\min_{(a,b) \in \mathbb{R}^2} \| Y - AX \|^2$$

Pythagorean theorem!

$$\|Y - z\|^2 = \|Y - z_0\|^2 + \|z - z_0\|^2$$

$$\geqslant \|Y - z_0\|^2$$

with equality if and only if $z = z_0$.



Explicit formulas

Projection matrix:

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

Solution of the least squares problem:

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

(so indeed $AX = PY$).

A proof of the formula for the projection matrix

$$z = P_{\mathrm{Im}\, A}(Y) \quad \text{iff} \quad \begin{cases} z \in \mathrm{Im}\, A \\ (Y - z) \in \underbrace{(\mathrm{Im}\ A)^{\perp}}_{\text{exercise! (they are equal subspaces)}} \end{cases}$$

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

exercise! (they are equal subspaces)

$$\underline{\text{i.e.}} \quad A^t(Y - AX) = 0$$

exercise! invertible if A has full rank

$$\text{i.e.} \quad A^t Y = A^t(AX) = \overbrace{(A^t A)}^{\text{invertible if } A \text{ has full rank}} X$$

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

$$\underline{\text{i.e}} \quad z = AX = A(A^t A)^{-1} A^t Y.$$