How to compute least square solutions of $A\mathbf{x} = \mathbf{b}$
(version 1.0)

1) Compute a basis of $\mathrm{Col}(A)$.

2) Use the Gram-Schmidt process to get an orthogonal basis of $\mathrm{Col}(A)$.

3) Use the orthogonal basis to compute $\mathrm{proj}_{\mathrm{Col}(A)}\mathbf{b}$.

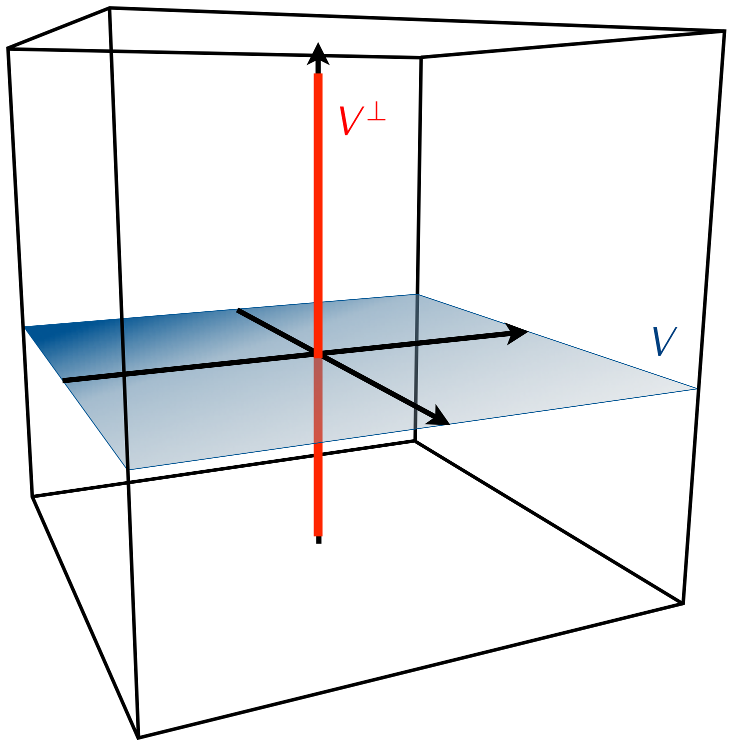
4) Compute solutions of the equation $A\mathbf{x} = \mathrm{proj}_{\mathrm{Col}(A)}\mathbf{b}$.

Next goal: Simplify this.

Definition

If V is a subspace of $\mathbb{R}^n$ then the *orthogonal complement* of V is the set $V^\perp$ of all vectors orthogonal to V:

$$V^\perp = \{\mathbf{w} \in \mathbb{R}^n \mid \mathbf{w} \cdot \mathbf{v} = 0\}$$



Propositon

If V is a subspace of $\mathbb{R}^n$ then:

1) $V^\perp$ is also a subspace of $\mathbb{R}^n$.
2) For each vector $\mathbf{w} \in \mathbb{R}^n$ there exist unique vectors $\mathbf{v} \in V$ and $\mathbf{z} \in V^\perp$ such that $\mathbf{w} = \mathbf{v} + \mathbf{z}$.

Definition

If A is an $m \times n$ matrix then the *row space* of A is the subspace $\mathrm{Row}(A)$ of $\mathbb{R}^n$ spanned by rows of A.

Example

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

Proposition

If A is a matrix then

$$\mathrm{Row}(A)^\perp = \mathrm{Nul}(A)$$

Corollary

If A is a matrix then

$$\mathrm{Col}(A)^{\perp} = \mathrm{Nul}(A^{T})$$

Back to least square solutions

Theorem

A vector $\hat{\mathbf{x}}$ is a least square solution of a matrix equation

$$A\mathbf{x} = \mathbf{b}$$

if and only if $\hat{\mathbf{x}}$ is an ordinary solution of the equation

$$(A^T A)\mathbf{x} = A^T\mathbf{b}$$

Theorem

The equation

$$(A^T A)\mathbf{x} = A^T\mathbf{b}$$

is called the *normal equation* of $A\mathbf{x} = \mathbf{b}$.

How to compute least square solutions of $A\mathbf{x} = \mathbf{b}$

(version 2.0)

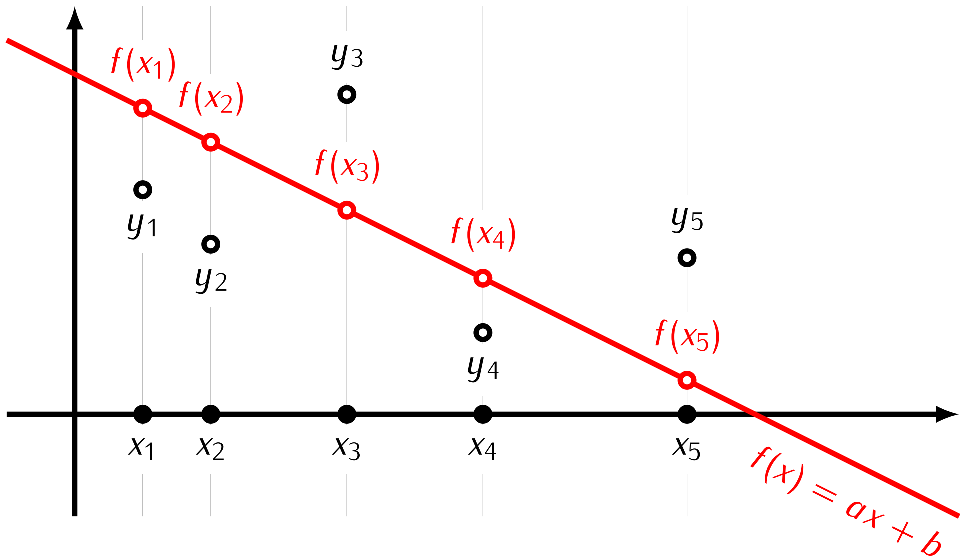
1) Compute $A^T A$, $A^T\mathbf{b}$.

2) Solve the normal equation $(A^T A)\mathbf{x} = A^T\mathbf{b}$.

Example. Compute least square solutions of the following equation:

$$\begin{bmatrix} 1 & 1 \\ 0 & 2 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

Application: Least square lines



Definition

If $(x_1, y_1), \ldots, (x_p, y_p)$ are points on the plane then the *least square line* for these points is the line given by an equation $f(x) = ax + b$ such that the number

$$\operatorname{dist}\left(\begin{bmatrix} y_1 \\ \vdots \\ y_p \end{bmatrix}, \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_p) \end{bmatrix}\right) = \sqrt{(y_1 - f(x_1))^2 + \ldots + (y_p - f(x_p))^2}$$

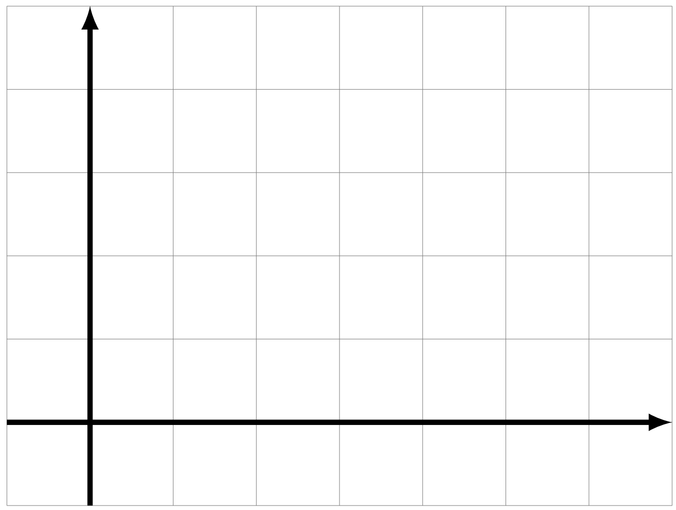
is the smallest possible.

Proposition

The line $f(x) = ax + b$ is the least square line for points $(x_1, y_1), \dots, (x_p, y_p)$ if the vector $\begin{bmatrix} a \\ b \end{bmatrix}$ is the least square solution of the equation

$$\begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_p & 1 \end{bmatrix} \cdot \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_p \end{bmatrix}$$

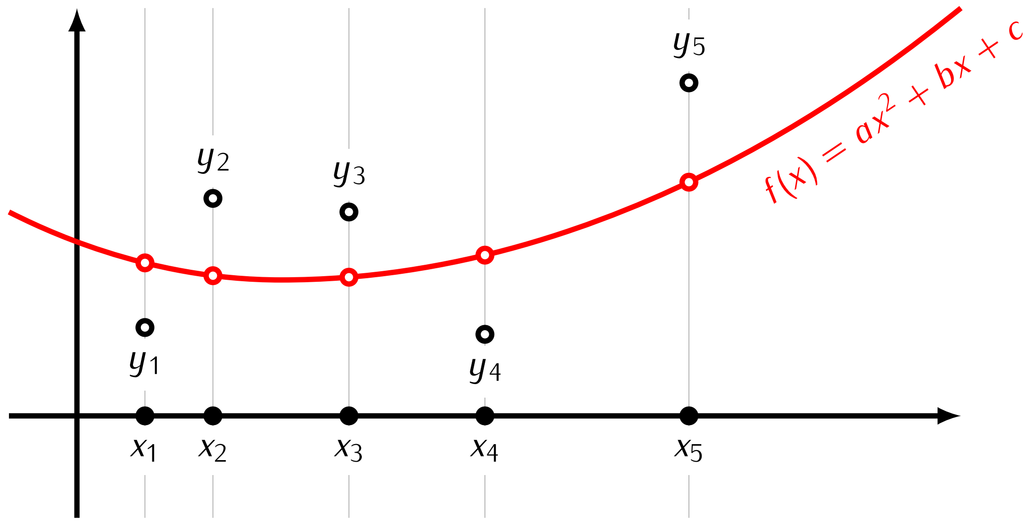
Example. Find the equation of the least square line for the points $(0, 0)$, $(1, 1)$, $(3, 1)$, $(5, 3)$.



Application: Least square curves

The above procedure can be used to determine curves other than lines that fit a set of points in the least square sense.

Example: Least square parabolas



Definition

If $(x_1, y_1), \ldots, (x_p, y_p)$ are points on the plane then the *least square parabola* for these points is the parabola given by an equation $f(x) = ax^2 + bx + c$ such that the number

$$\operatorname{dist}\left(\begin{bmatrix} y_1 \\ \vdots \\ y_p \end{bmatrix}, \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_p) \end{bmatrix}\right) = \sqrt{(y_1 - f(x_1))^2 + \ldots + (y_p - f(x_p))^2}$$

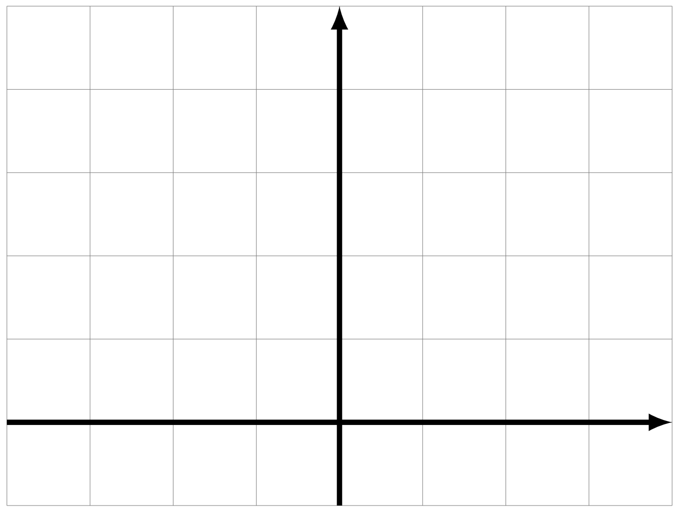
is the smallest possible.

Proposition

The parabola $f(x) = ax^2 + bx + c$ is the least square parabola for points $(x_1, y_1), \ldots, (x_p, y_p)$ if the vector $\begin{bmatrix} a \\ b \\ c \end{bmatrix}$ is the least square solution of the equation

$$\begin{bmatrix} x_1^2 & x_1 & 1 \\ \vdots & \vdots & \\ x_p^2 & x_p & 1 \end{bmatrix} \cdot \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_p \end{bmatrix}$$

Example. Find the equation of the least square parabola for the points $(-2, 2)$, $(0, 0)$, $(1, 1)$, $(2, 3)$.



Recall:

1) The dot product in $\mathbb{R}^n$:

$$\begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} \cdot \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix} = a_1b_1 + a_2b_2 + \ldots a_nb_n$$

2) Properties of the dot product:

a) $\mathbf{u} \cdot \mathbf{v} = \mathbf{v} \cdot \mathbf{u}$

b) $(\mathbf{u} + \mathbf{v}) \cdot \mathbf{w} = \mathbf{u} \cdot \mathbf{w} + \mathbf{v} \cdot \mathbf{w}$

c) $(c\mathbf{u}) \cdot \mathbf{v} = c(\mathbf{u} \cdot \mathbf{v})$

d) $\mathbf{u} \cdot \mathbf{u} \geq 0$ and $\mathbf{u} \cdot \mathbf{u} = 0$ if and only if $\mathbf{u} = \mathbf{0}$.

2) Using the dot product we can define:

- length of vectors
- distance between vectors
- orthogonality of vectors
- orthogonal and orthonormal bases
- orthogonal projection of a vector onto a subspace of $\mathbb{R}^n$
- ...

Next: Generalization to arbitrary vector spaces.