

Lesson 11

*Or how to find a
near solution of
inconsistent systems*

Chapter 6 Orthogonality and least squares

► Inner Product, Length and Orthogonality

► Orthogonal Sets

► Orthogonal Projections

► The Gram-Schmidt Process

► Least-Squares Problems

► Applications to Linear Models

► Inner Product Spaces

► Applications of Inner Product Spaces

OPGAVE 2 (fra lektion 10)

Matricen A her er tæt på at være ortogonal

- Hvad vil det sige, at en matrix er ortogonal?
- "Reparer" på A, således at den bliver ortogonal
hint: kig på elementet med indeks 3,2

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$



Søjlevektorerne (og rækkevektorerne) er indbyrdes ortogonale – MEN:

Definition:

Søjler og rækker skal også være *normale* for at vi siger, at matricen A er ortogonal.

$$A = \begin{bmatrix} 0.707 & 0.707 & 0 \\ 0.707 & -0.707 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Inner product (dot product): $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^T \mathbf{v} = [u_1 \ u_2 \ \cdots \ u_n] \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = u_1 v_1 + u_2 v_2 + \cdots + u_n v_n = \sum_{i=1}^n u_i v_i \in \mathbb{R}$$

- $\mathbf{u} \cdot \mathbf{v} = \mathbf{v} \cdot \mathbf{u}$
- $(\mathbf{u} + \mathbf{v}) \cdot \mathbf{w} = \mathbf{u} \cdot \mathbf{w} + \mathbf{v} \cdot \mathbf{w}$
- $(c\mathbf{u}) \cdot \mathbf{v} = \mathbf{u} \cdot (c\mathbf{v})$
- $\mathbf{u} \cdot \mathbf{u} \geq 0$ and $\mathbf{u} \cdot \mathbf{u} = 0 \iff \mathbf{u} = \mathbf{0}$
- The **norm** (or length) of a vector is defined as: $\|\mathbf{v}\| = \sqrt{\mathbf{v} \cdot \mathbf{v}} = \sqrt{v_1^2 + \cdots + v_n^2}$
- A vector \mathbf{v} is **normalized** (unit vector) if: $\|\mathbf{v}\| = 1$
- The **distance** between two vectors is defined as:
$$\text{dist}(\mathbf{u}, \mathbf{v}) = \|\mathbf{u} - \mathbf{v}\| = \sqrt{(u_1 - v_1)^2 + \cdots + (u_n - v_n)^2}$$
- The **angle** θ between two vectors is given by: $\mathbf{u} \cdot \mathbf{v} = \|\mathbf{u}\| \|\mathbf{v}\| \cos(\theta)$

Definitions

Orthogonal set

A set of vectors $S = \{\mathbf{u}_1 \cdots \mathbf{u}_n\}$ in \mathbb{R}^n with $\mathbf{u}_i \perp \mathbf{u}_j$ for all $i \neq j$

That is: $\mathbf{u}_i \cdot \mathbf{u}_j = 0$ for all $i \neq j$

Orthonormal set

An orthogonal set of vectors $S = \{\mathbf{u}_1 \cdots \mathbf{u}_n\}$ in \mathbb{R}^n with $\|\mathbf{u}_i\| = 1$ for all $i = 1, \dots, n$.

That is: $\mathbf{u}_i \cdot \mathbf{u}_j = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$

Orthogonal complement W^\perp

The set of all vectors in \mathbb{R}^n which are orthogonal to all vectors in W .

Theorem 6.8 - The Orthogonal Decomposition Theorem

Let $\{\mathbf{u}_1 \cdots \mathbf{u}_n\}$ be an orthogonal basis of \mathbb{R}^n .

For each \mathbf{y} in \mathbb{R}^n :

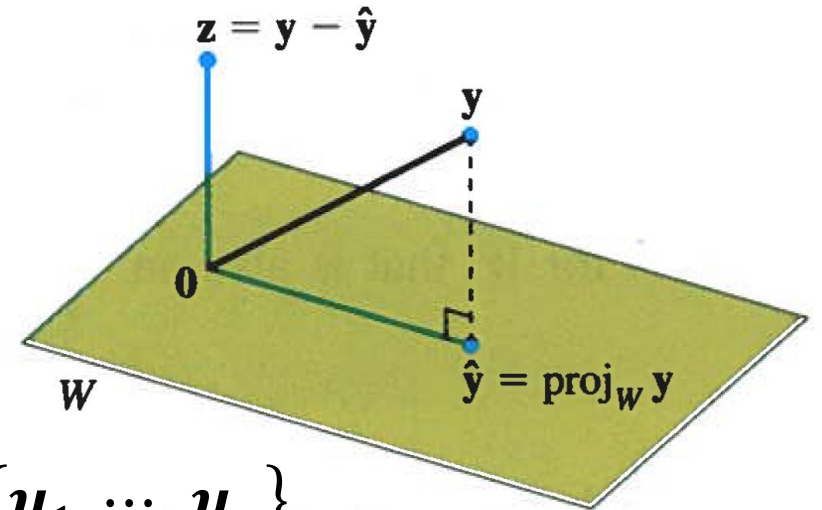
$$\mathbf{y} = c_1 \mathbf{u}_1 + \cdots + c_n \mathbf{u}_n = \hat{\mathbf{y}} + \mathbf{z}$$

where

$$\hat{\mathbf{y}} = \frac{\mathbf{y} \cdot \mathbf{u}_1}{\mathbf{u}_1 \cdot \mathbf{u}_1} \mathbf{u}_1 + \cdots + \frac{\mathbf{y} \cdot \mathbf{u}_p}{\mathbf{u}_p \cdot \mathbf{u}_p} \mathbf{u}_p = \text{proj}_W \mathbf{y} \in W = \text{Span}\{\mathbf{u}_1, \dots, \mathbf{u}_p\}$$

$$\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}} = \frac{\mathbf{y} \cdot \mathbf{u}_{p+1}}{\mathbf{u}_{p+1} \cdot \mathbf{u}_{p+1}} \mathbf{u}_{p+1} + \cdots + \frac{\mathbf{y} \cdot \mathbf{u}_n}{\mathbf{u}_n \cdot \mathbf{u}_n} \mathbf{u}_n = \text{proj}_{W^\perp} \mathbf{y} \in W^\perp = \text{Span}\{\mathbf{u}_{p+1}, \dots, \mathbf{u}_n\}$$

$$\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}} \perp \hat{\mathbf{y}}$$

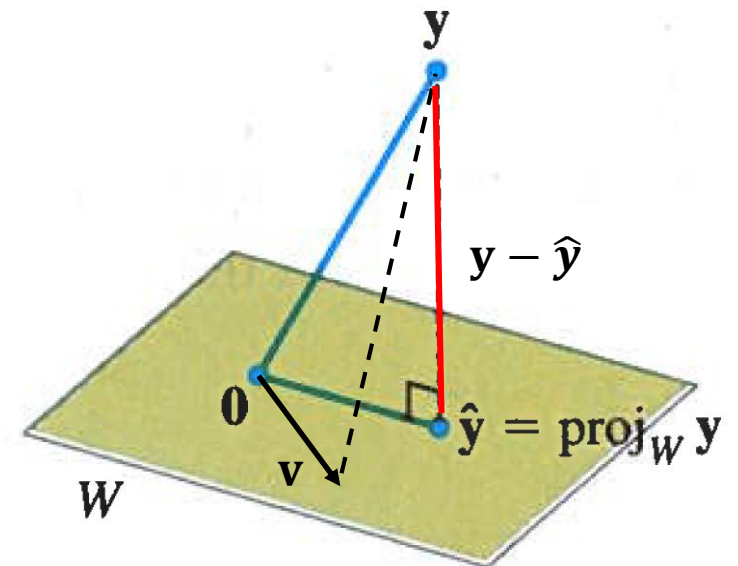


Theorem 6.9: The Best Approximation Theorem

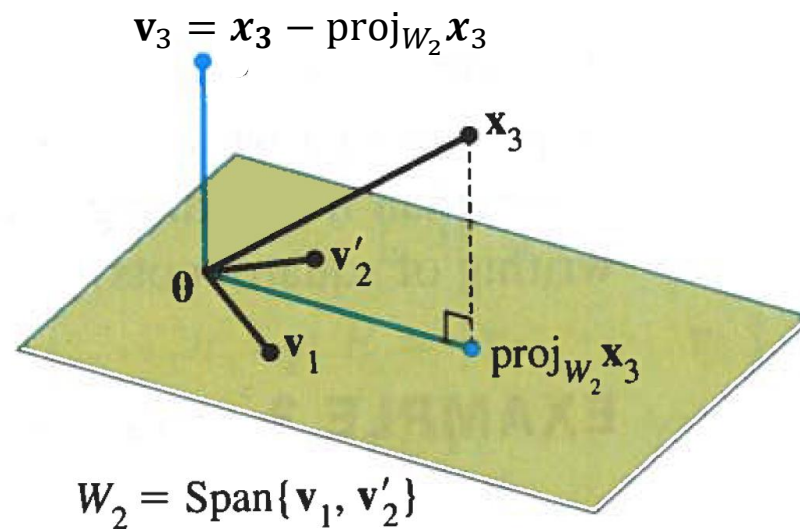
Let W be a subspace of \mathbb{R}^n , let \mathbf{y} be any vector in \mathbb{R}^n , and let $\hat{\mathbf{y}}$ be the orthogonal projection of \mathbf{y} onto W . Then $\hat{\mathbf{y}}$ is the closest point in W to \mathbf{y} in the sense that

$$\|\mathbf{y} - \hat{\mathbf{y}}\| < \|\mathbf{y} - \mathbf{v}\|$$

for all \mathbf{v} in W distinct from $\hat{\mathbf{y}}$.



6.4 The Gram-Schmidt Process

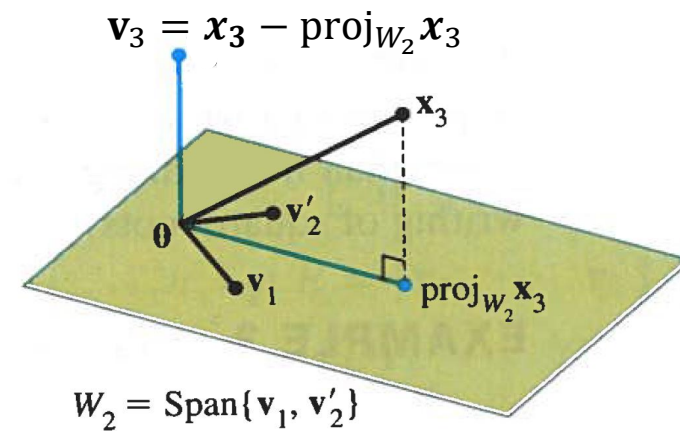
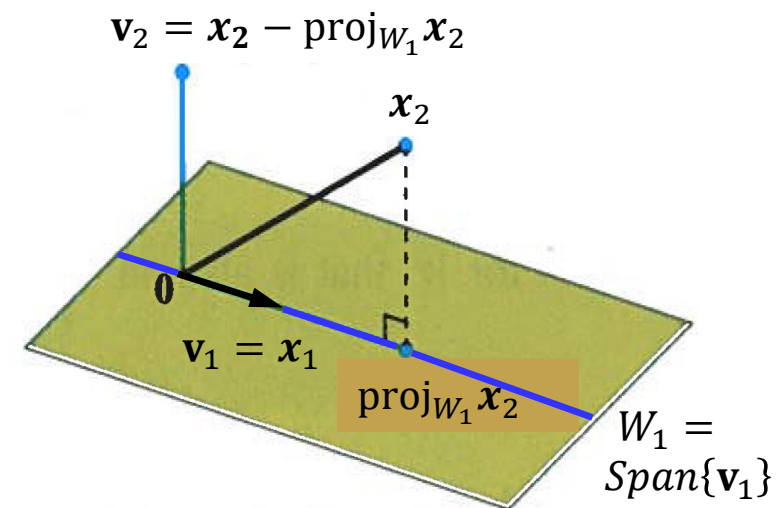


Ex 1

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\mathbf{x}_2 = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$



The Gram-Schmidt Process

Given a basis $\{\mathbf{x}_1, \dots, \mathbf{x}_p\}$ for a subspace W of \mathbb{R}^n . Define:

$$\mathbf{v}_1 = \mathbf{x}_1$$

$$\mathbf{v}_2 = \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1$$

$$\mathbf{v}_3 = \mathbf{x}_3 - \frac{\mathbf{x}_3 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 - \frac{\mathbf{x}_3 \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \mathbf{v}_2$$

$$\vdots$$

$$\mathbf{v}_p = \mathbf{x}_p - \frac{\mathbf{x}_p \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 - \frac{\mathbf{x}_p \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \mathbf{v}_2 - \dots - \frac{\mathbf{x}_p \cdot \mathbf{v}_{p-1}}{\mathbf{v}_{p-1} \cdot \mathbf{v}_{p-1}} \mathbf{v}_{p-1}$$

Then $\{\mathbf{v}_1, \dots, \mathbf{v}_p\}$ is an orthogonal basis for W ,

and $\text{Span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\} = \text{Span}\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ for $k = 1, \dots, p$

Theorem 6.12: The QR Factorization

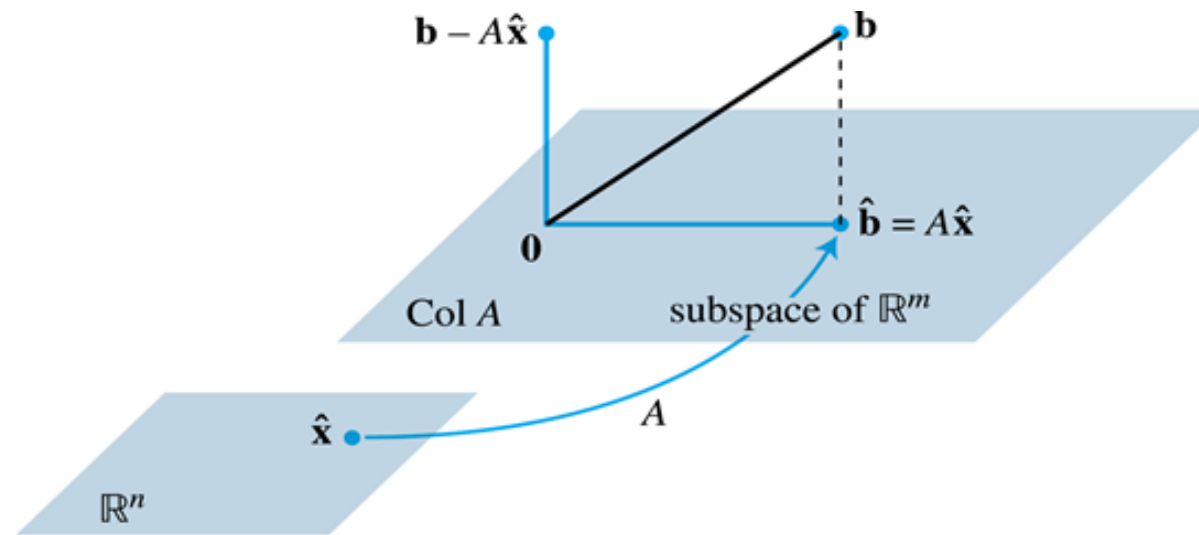
If A is an $m \times n$ matrix with linearly independent columns, then A can be factored as:

$$A = QR$$

where

- Q is an $m \times n$ matrix whose columns form an orthonormal basis for $\text{Col } A$
- R is an $n \times n$ upper triangle invertible matrix with positive entries on its diagonal.

6.5 Least Squares Problems



Least-squares problems

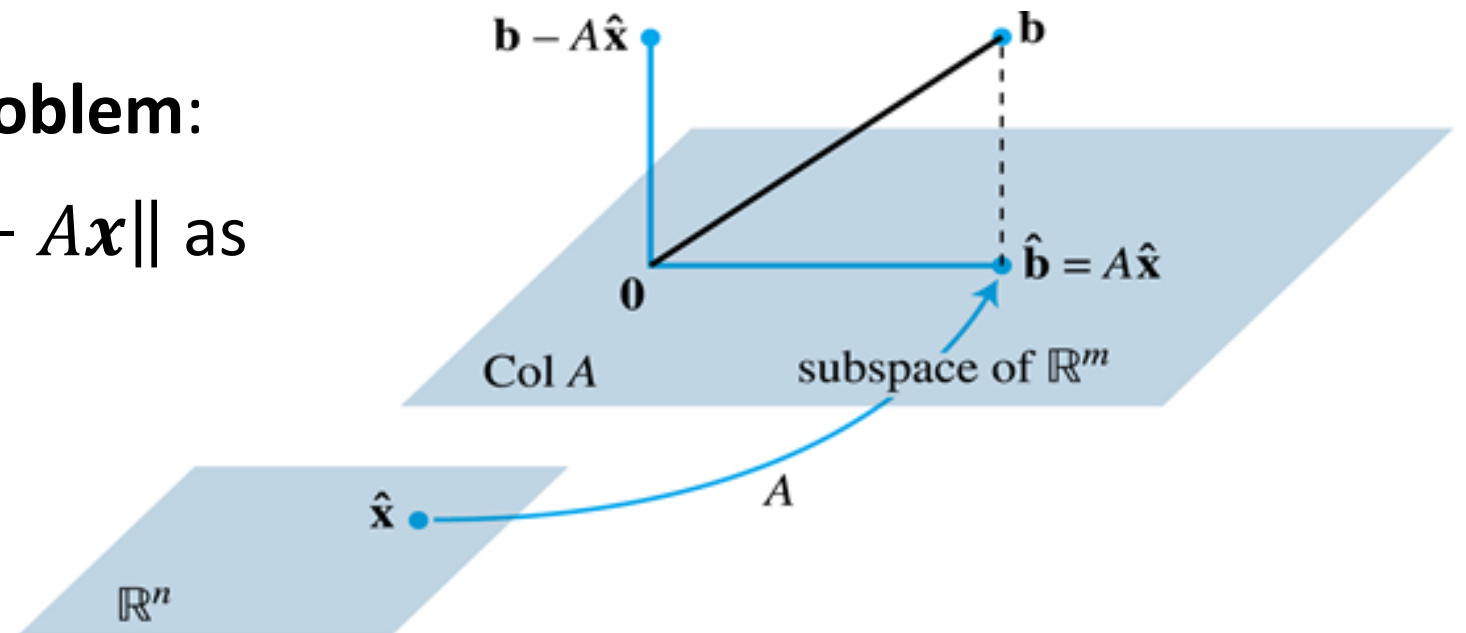
Often – in real life – $A\mathbf{x} = \mathbf{b}$ has no solutions (are inconsistent).

That is, $\mathbf{b} \notin \text{Col } A$.

The best approximation of \mathbf{b} is the vector in $\text{Col } A$, that is closest to \mathbf{b} .

The general least-squares problem:

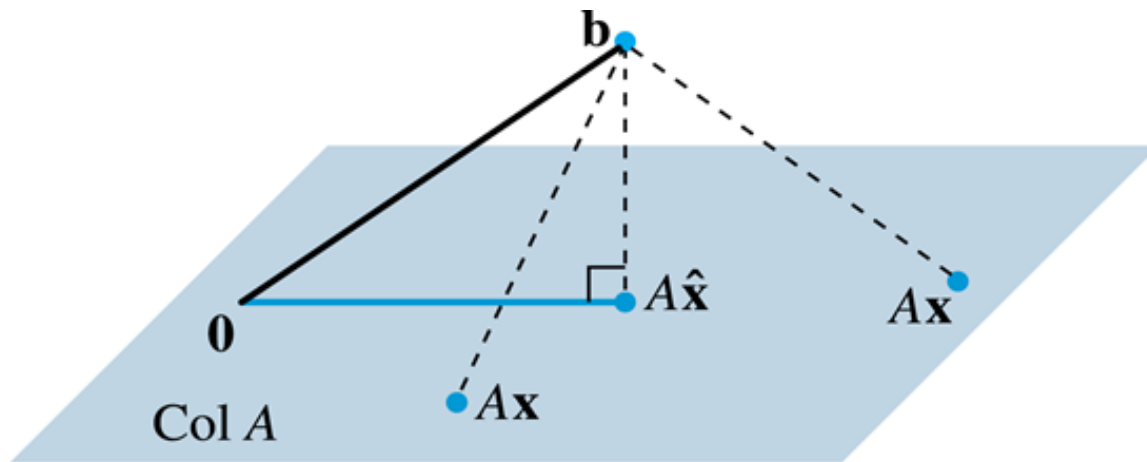
- Find an \mathbf{x} that makes $\|\mathbf{b} - A\mathbf{x}\|$ as small as possible,



Definition:

Let A be an $m \times n$ matrix and let \mathbf{b} be in \mathbb{R}^m . A least squares solution of $A\mathbf{x} = \mathbf{b}$ is then $\hat{\mathbf{x}}$ in \mathbb{R}^n such that

$$\|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|, \quad \forall \mathbf{x} \in \mathbb{R}^n$$



By Theorem 6.9:

$$A\hat{\mathbf{x}} = \text{proj}_{\text{Col } A} \mathbf{b} = \hat{\mathbf{b}}$$

$$A\hat{\mathbf{x}} = \hat{\mathbf{b}} = \text{proj}_{\text{Col } A} \mathbf{b}$$

\Leftrightarrow

$$(\mathbf{b} - A\hat{\mathbf{x}}) \perp \text{Col } A = \text{Span}\{\mathbf{a}_1, \dots, \mathbf{a}_n\}$$

\Leftrightarrow

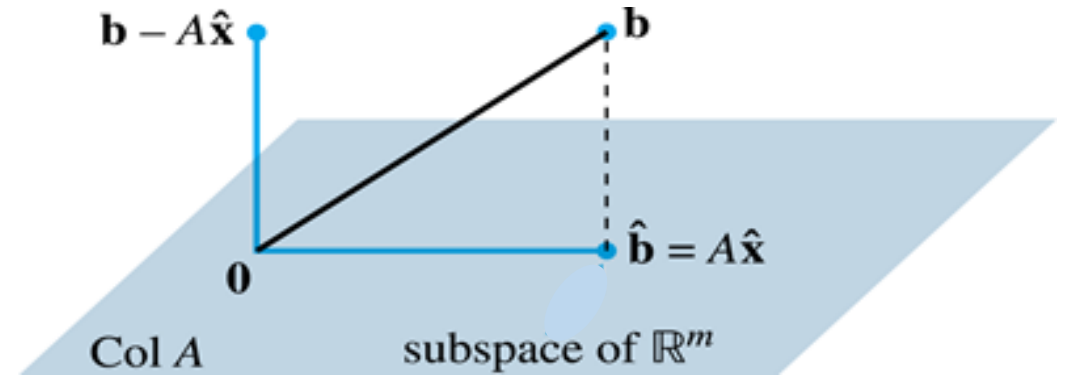
$$\mathbf{a}_j \cdot (\mathbf{b} - A\hat{\mathbf{x}}) = \mathbf{a}_j^T (\mathbf{b} - A\hat{\mathbf{x}}) = 0 \quad \text{where } \mathbf{a}_j \text{ is any column of } A = [\mathbf{a}_1 \cdots \mathbf{a}_n]$$

\Leftrightarrow

$$A^T (\mathbf{b} - A\hat{\mathbf{x}}) = \mathbf{0}$$

\Leftrightarrow

$$A^T A \hat{\mathbf{x}} = A^T \mathbf{b}$$



Theorem 6.13: The Normal Equations

The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ coincides with the nonempty set of solutions of the normal equations $A^T A\mathbf{x} = A^T \mathbf{b}$

Diskussion:

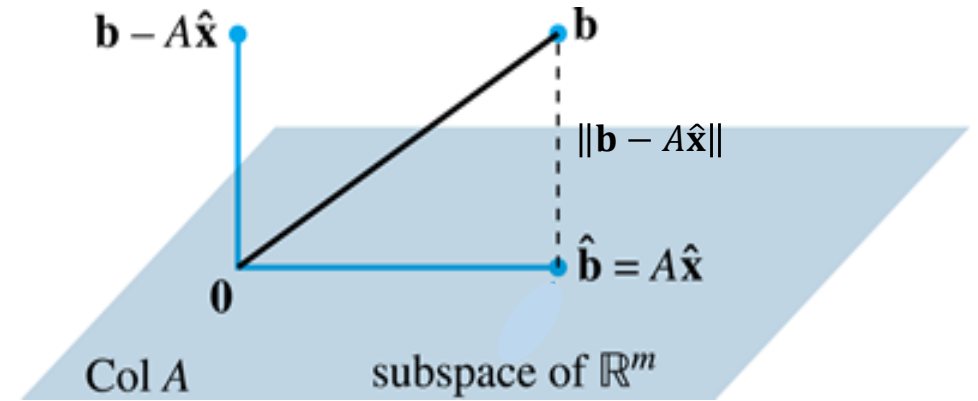
Givet A er en $m \times n$ matrix – hvilken dimension har så $A^T A$?
Hvad skal der mon til for at finde \mathbf{x} ?

$$\mathbf{x} = (A^T A)^{-1} A^T \mathbf{b}$$

Matricen foran \mathbf{b} kaldes:
More-Penrose pseudo-inverse

Ex 4

$$A = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}$$



Dette er et *overbestemt* ligningssystem -
kendetegnet ved flere ligninger end ubekendte

Ved løsning af normalligningerne
finder vi den *bedst mulige* løsning:

$$\hat{\mathbf{x}} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

Least-squares error: $\|\mathbf{b} - A\hat{\mathbf{x}}\|$

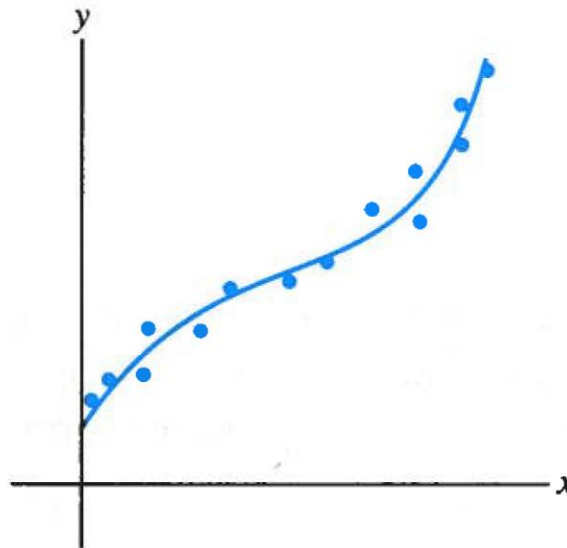
OPGAVE 1

For det overbestemte ligningssystem $A\mathbf{x} = \mathbf{b}$, hvor:

$$A = \begin{bmatrix} 3 & -2 \\ -3 & 1 \\ -1 & 4 \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} 6 \\ 1 \\ 9 \end{bmatrix}$$

- Bestem den pseudo-inverse matrix
- Find det \mathbf{x} , som i mindste kvadraters forstand bedst muligt approximere \mathbf{b} , når multipliceret med A
- Udregn LSE (least squares error)

6.6 Applications to Linear Models



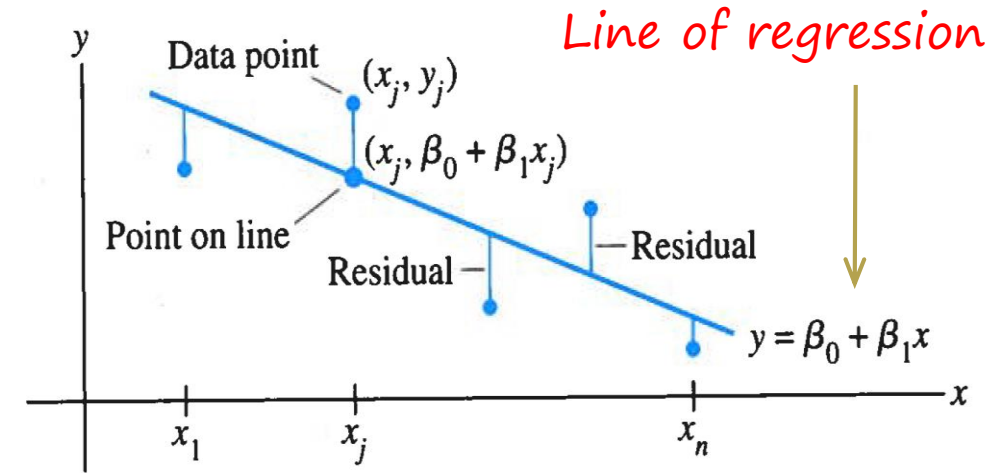
Least-Squares Lines

Fitting data to a straight line:

$$y = \beta_0 + \beta_1 x$$

\hat{y} →

Predicted y-value	Observed y-value
$\beta_0 + \beta_1 x_1$	y_1
$\beta_0 + \beta_1 x_2$	y_2
\vdots	\vdots
$\beta_0 + \beta_1 x_n$	y_n



Data points: $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i = \hat{y}_i + \varepsilon_i$, where $\hat{y}_i = \beta_0 + \beta_1 x_i$ is the predicted y-value

Residual (error): $\varepsilon_i = y_i - (\beta_0 + \beta_1 x_i) = y_i - \hat{y}_i$

Determine the unknown parameters β_0 and β_1 that minimize the sum of square residuals:

$$\sum_{i=1}^n \varepsilon_i^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \|\mathbf{y} - \hat{\mathbf{y}}\|^2$$

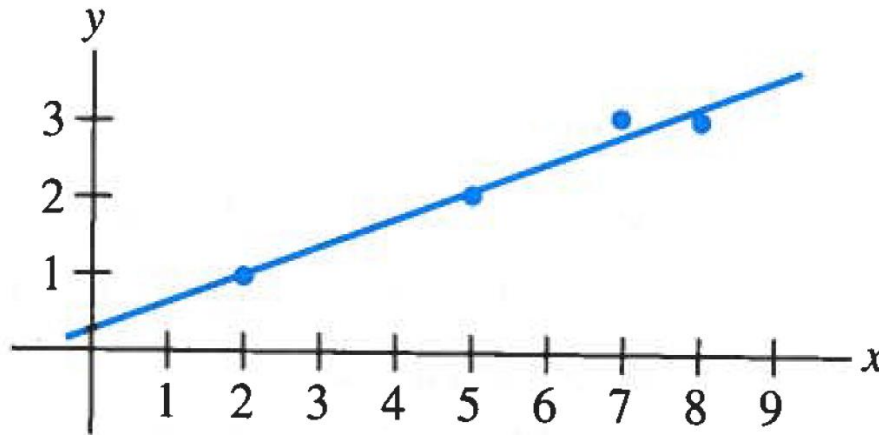
That is, find a least-squares solution of $X\boldsymbol{\beta} = \mathbf{y}$, where $X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$, $\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$ and $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$

Ex 5

Data points: $(x_i, y_i) = (2,1), (5,2), (7,3), (8,3) \rightarrow y = \beta_0 + \beta_1 x$

Beregning:

Bestem de koefficienter β_0 og β_1 , som for en ret linje giver den bedste approximation til datasættet.

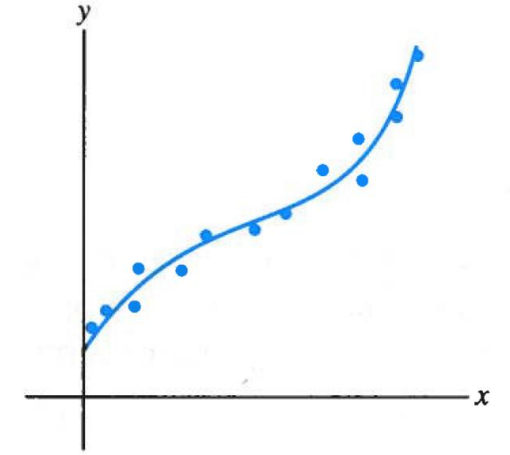


$$\begin{aligned}\beta_0 &= 0.286 \\ \beta_1 &= 0.357\end{aligned}$$

Least-Squares fitting

Fitting data to polynomium: $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$

Data points: $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$



Determine the unknown parameters β_0, \dots, β_3 that minimize the sum of square residuals:

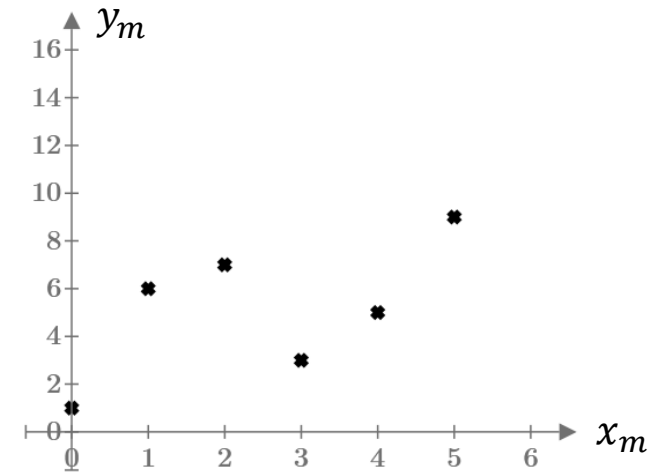
$$\sum_{i=1}^n \varepsilon_i^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \|\mathbf{y} - \hat{\mathbf{y}}\|^2, \quad \hat{\mathbf{y}} = X\boldsymbol{\beta}$$

That is, find a least-squares solution of: $X\boldsymbol{\beta} = \mathbf{y}$

	Observation vector	Design matrix	Parameter vector	Residual vector
where:	$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$	$X = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 \end{bmatrix}$	$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}$	$\boldsymbol{\varepsilon} = \mathbf{y} - \hat{\mathbf{y}} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$

Ex 6

Data points: $x_m := \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$ $y_m := \begin{bmatrix} 1 \\ 6 \\ 7 \\ 3 \\ 5 \\ 9 \end{bmatrix}$



Fitting curve: $f(x) = \beta_0 + \beta_1 \cdot x + \beta_2 \cdot x^2 + \beta_3 \cdot x^3$

Parameter vector: $\beta := \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}$

Design matrix: $X := \begin{bmatrix} x_m^0 & x_m^1 & x_m^2 & x_m^3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 8 \\ 1 & 3 & 9 & 27 \\ 1 & 4 & 16 & 64 \\ 1 & 5 & 25 & 125 \end{bmatrix}$

\Downarrow

$$X^T = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 & 5 \\ 0 & 1 & 4 & 9 & 16 & 25 \\ 0 & 1 & 8 & 27 & 64 & 125 \end{bmatrix} \Rightarrow X^T X = \begin{bmatrix} 6 & 15 & 55 & 225 \\ 15 & 55 & 225 & 979 \\ 55 & 225 & 979 & 4425 \\ 225 & 979 & 4425 & 20515 \end{bmatrix}$$

Ex 6

Normal equation: $X^T X \cdot \beta = X^T y_m \Rightarrow$

$$\begin{bmatrix} 6 & 15 & 55 & 225 \\ 15 & 55 & 225 & 979 \\ 55 & 225 & 979 & 4425 \\ 225 & 979 & 4425 & 20515 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 & 5 \\ 0 & 1 & 4 & 9 & 16 & 25 \\ 0 & 1 & 8 & 27 & 64 & 125 \end{bmatrix} \begin{bmatrix} 1 \\ 6 \\ 7 \\ 3 \\ 5 \\ 9 \end{bmatrix} = \begin{bmatrix} 31 \\ 94 \\ 366 \\ 1588 \end{bmatrix}$$

Augmented matrix: $A_{aug} = [X^T X; X^T y_m] =$

$$\begin{bmatrix} 6 & 15 & 55 & 225 & 31 \\ 15 & 55 & 225 & 979 & 94 \\ 55 & 225 & 979 & 4425 & 366 \\ 225 & 979 & 4425 & 20515 & 1588 \end{bmatrix}$$

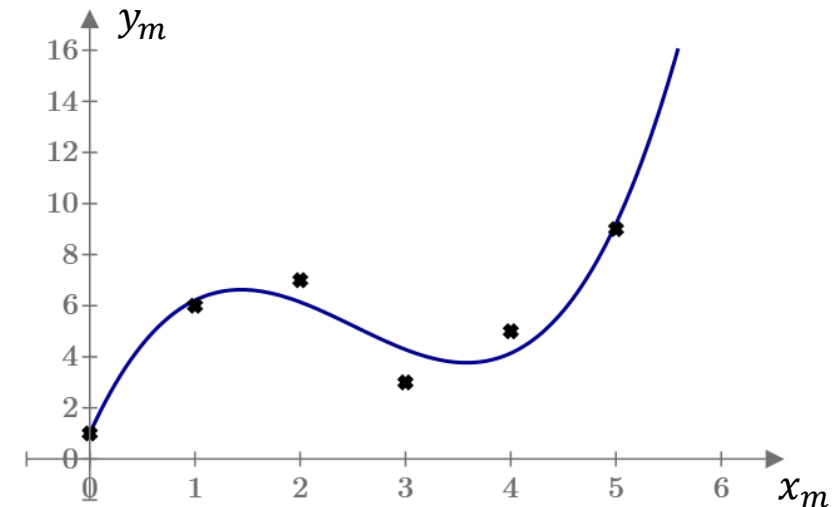
Reduced echelon form: $A_{rref} := \text{rref}(A_{aug}) =$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 9.024 \\ 0 & 0 & 1 & 0 & -4.393 \\ 0 & 0 & 0 & 1 & 0.583 \end{bmatrix} \Rightarrow \beta := \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 9.024 \\ -4.393 \\ 0.583 \end{bmatrix}$$

Best regression curve: $f(x) := 1 + 9.024 \cdot x - 4.393 \cdot x^2 + 0.583 \cdot x^3$

Residuals (errors): $\varepsilon := y_m - f(x_m) =$

$$\begin{bmatrix} 0 \\ -0.214 \\ 0.857 \\ -1.286 \\ 0.857 \\ -0.214 \end{bmatrix} \quad \|\varepsilon\| = 1.793$$



Vi har som eksempel et datasæt (x,y) , som vi ønsker approximeret med en parabolisk funktion

$$y = ax^2 + bx + c$$

Det første datapar (x,y) er $(2,3)$

Diskussion:

Hvilke talværdier består første række af designmatricen af?

Første række i designmatricen må være $[1 \ 2 \ 4]$

Least-Squares fitting of other curves

Fitting data to known functions: $y = \beta_0 f_0(x) + \beta_1 f_1(x) + \cdots + \beta_k f_k(x)$

Known (fitting)
functions

Linear model =
Linear in the
unknown
parameters β_i

Data points: $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$

Determine the unknown parameters β_0, \dots, β_k that minimize the sum of square residuals:

$$\sum_{i=1}^n \varepsilon_i^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \|\mathbf{y} - \hat{\mathbf{y}}\|^2, \quad \hat{\mathbf{y}} = X\boldsymbol{\beta}$$

That is, find a least-squares solution of: $X\boldsymbol{\beta} = \mathbf{y}$

Observation
vector

Design
matrix

Parameter
vector

Residual
vector

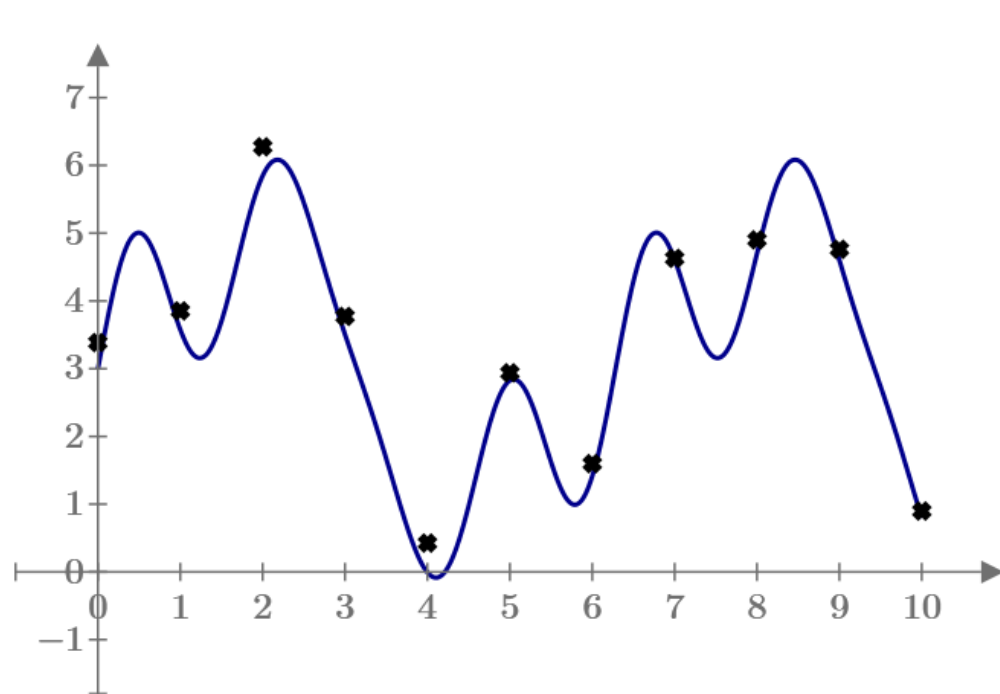
where:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad X = \begin{bmatrix} f_0(x_1) & f_1(x_1) & \cdots & f_k(x_1) \\ f_0(x_2) & f_1(x_2) & \cdots & f_k(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_0(x_n) & f_1(x_n) & \cdots & f_k(x_n) \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} \quad \boldsymbol{\varepsilon} = \mathbf{y} - \hat{\mathbf{y}} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

Ex 7 Least-Squares fitting of sinusoidal harmonics

Fitting functions: $f_0(x) = 1$; $f_1(x) = \sin(x)$; $f_2(x) = \sin(2x)$; ... ; $f_k(x) = \sin(kx)$

Fitting curve: $y = \beta_0 + \beta_1 \sin(x) + \beta_2 \sin(2x) + \cdots + \beta_k \sin(kx)$



Harmonic/Fourier series

Today's words and concepts

Least-squares solution

Gram-Schmidt process

The normal equation

Least-squares error

Residual

Least-squares fitting

Observation vector

Design matrix

Parameter vector

Residual vector

Least-squares lines

QR factorization