Math 504 (Fall 2010) - Lecture 12

Householder Triangularization and Least Squares Problem

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Outline

- QR factorization by Householder reflectors - Lecture 10
  - Algorithm
  - Operation count
- Least squares - Lecture 11
  - Problem definition
  - Numerical solution by QR factorization
  - Normal equations

QR factorization by HH reflectors, Algorithm

<u>Step k of the algorithm:</u> ($k = 1, \ldots, n-1$)

$$\underbrace{\begin{bmatrix} R & B \\ 0 & A^{(k)} \end{bmatrix}}_{Q_{k-1} \ldots Q_1 A} \longrightarrow \underbrace{\begin{bmatrix} R & B \\ 0 & \hat{Q}_k A^{(k)} \end{bmatrix}}_{Q_k Q_{k-1} \ldots Q_1 A}$$

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- $Q_k = \begin{bmatrix} I_{k-1} & 0 \\ 0 & \hat{Q}_k \end{bmatrix} \in \mathbb{C}^{m\times m}$, $R \in \mathbb{C}^{(k-1)\times(k-1)}$ is upper triangular

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- $\hat{Q}_k \in \mathbb{C}^{(m-k+1)\times(m-k+1)}$ is the HH reflector assoc with $a_1^{(k)}$ so that

$$A^{(k)} = \begin{bmatrix} x & x & x & \ldots & x \\ x & x & x & \ldots & x \\ \vdots & \vdots & & & \vdots \\ x & x & x & \ldots & x \end{bmatrix} \longrightarrow \hat{Q}_k A^{(k)} = \begin{bmatrix} x & x & x & \ldots & x \\ 0 & x & x & \ldots & x \\ \vdots & \vdots & & & \vdots \\ 0 & x & x & \ldots & x \end{bmatrix}$$

QR factorization by HH reflectors, Algorithm

ALGORITHM

Input: $A \in \mathbb{C}^{m \times n}$ with $m \geq n$

Output: Upper triangular $R \in \mathbb{C}^{m \times n}$ and the HH vectors $u_1, \ldots, u_{n-1} \in \mathbb{C}^m$. The unitary factor $Q \in \mathbb{C}^{m \times m}$ can be formed from the HH vectors so that $A = QR$ is a full QR factorization.

for $k = 1, n$ **do**

$v \leftarrow A_{k:m,k}$

$u_k \leftarrow v - \|v\| e_1$

$u_k \leftarrow u_k / \|u_k\|$

$A_{k:m,k:n} \leftarrow A_{k:m,k:n} - 2u_k(u_k^* A_{k:m,k:n})$

end for

$R \leftarrow A$

Return R

QR factorization by HH reflectors, Algorithm

The unitary factor Q such that $A = QR$ can be recovered from the HH vectors u_k.

QR factorization by HH reflectors, Algorithm

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equivalently

$$A = Q_1^* Q_2^* \cdots Q_n^* R = \underbrace{Q_1 Q_2 \cdots Q_n}_{Q} R.$$

QR factorization by HH reflectors, Algorithm

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QR factorization by HH reflectors, Algorithm

- A very common use of the QR factorization is the numerical solution of the least squares problem.

- For the least squares problem Q does not need to be formed explicitly. Given $b \in \mathbb{C}^m$. We will need the product $Q^* b$, which can be computed by means of the vectors u_k, since

$$Q_k^* b = \underbrace{\begin{bmatrix} I_{k-1} & 0 \\ 0 & I_{m-k+1} - 2u_k u_k^* \end{bmatrix}}_{Q_k^* = Q_k} \underbrace{\begin{bmatrix} \hat{b} \in \mathbb{C}^{k-1} \\ \tilde{b} \in \mathbb{C}^{m-k+1} \end{bmatrix}}_{b} = \begin{bmatrix} \hat{b} \\ \tilde{b} - 2u_k(u_k^* \tilde{b}) \end{bmatrix}.$$

QR factorization by HH reflectors, Algorithm

Remarks

- The algorithm based on HH reflectors shows the existence of a QR factorization.

> Theorem (Existence of a QR factorization)
> Every matrix $A \in \mathbb{C}^{m \times n}$ with $m \geq n$ has a QR factorization.

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- Pay attention to the order of operation to perform $2u_k u_k^* A_{k:m,k:n}$.

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  - Inefficient way: $2(u_k u_k^*)A_{k:m,k:n}$

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    $\#FLOPS = 3(m-k+1) \times (n-k+1) + O(n)$

QR factorization by HH reflectors, Operation Count

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QR factorization by HH reflectors, Operation Count

$$
\begin{aligned}
\text{Total }\#\text{ FLOPS} &= \sum_{k=1}^{n} \left(4(m-k+1)(n-k+1) + O(m) + O(n)\right) \\
&= 4\left(mn^2 - m\frac{n(n+1)}{2} - n\frac{n(n+1)}{2} + \frac{n(n+1)(2n+1)}{6}\right) \\
&\qquad + O(mn) + O(n^2) \\
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(Recall that Gram-Schmidt requires $2mn^2$ flops.)

QR factorization by HH reflectors, Operation Count

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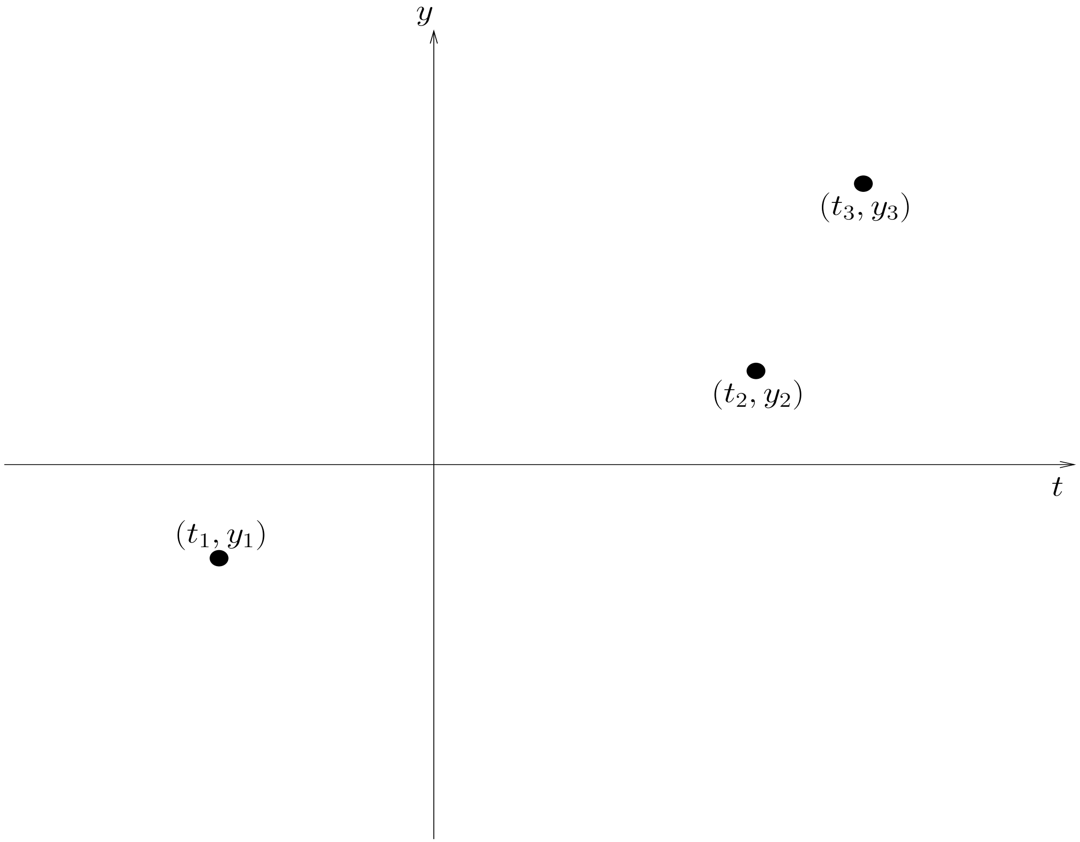
Least Squares, Problem Definition

Given $p_1 = (t_1, y_1) = (-2, -1)$, $p_2 = (t_2, y_2) = (3, 1)$, $p_3 = (t_3, y_3) = (4, 3)$.



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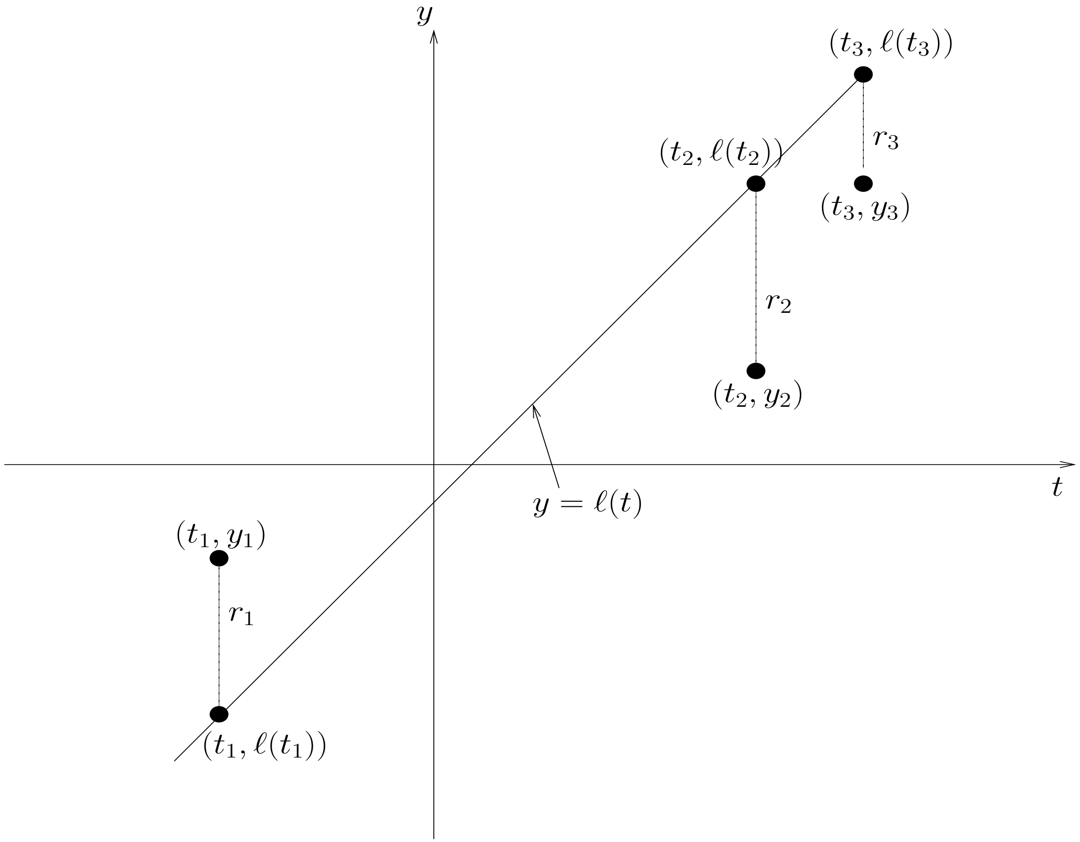

- Find the line $\ell(t) = x_1 t + x_0$ that best fits the points p_1, p_2, p_3. (The unknowns are x_0, x_1.)

Least Squares, Problem Definition

- Find the line $\ell(t) = x_1 t + x_0$ so that

$$\sqrt{\sum_{i=1}^{3} (\ell(t_i) - y_i)^2} = \sqrt{(-2x_1 + x_0 - (-1))^2 + (3x_1 + x_0 - 1)^2 + (4x_1 + x_0 - 3)^2}$$

is small as possible.

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$$r = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} = \begin{bmatrix} \ell(t_1) - y_1 \\ \ell(t_2) - y_2 \\ \ell(t_3) - y_3 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & -2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_0 \\ x_1 \end{bmatrix}}_{x} - \underbrace{\begin{bmatrix} -1 \\ 1 \\ 3 \end{bmatrix}}_{b}$$

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- The problem can be posed as

  find $x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix}$ such that $\|r\|_2 = \|Ax - b\|_2$ is as small as possible.

Least Squares, Problem Definition

- More generally given m points in $\mathbf{R}^2$

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- Suppose you want to find the polynomial of degree $n-1$ $(n < m)$ in the form

$$P(t) = x_{n-1}t^{n-1} + x_{n-2}t^{n-2} + \cdots + x_1 t + x_0$$

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minimizing

$$\sqrt{\sum_{i=1}^{m} (p(t_i) - y_i)^2}.$$

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- Define

$$\underbrace{\begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_m \end{bmatrix}}_{r} = \begin{bmatrix} P(t_1) - y_1 \\ P(t_2) - y_2 \\ \vdots \\ P(t_m) - y_m \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & \cdots & t_1^{n-2} & t_1^{n-1} \\ 1 & \cdots & t_2^{n-2} & t_2^{n-1} \\ & & \vdots & \vdots \\ 1 & \cdots & t_m^{n-2} & t_m^{n-1} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{bmatrix}}_{x} - \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}}_{b}$$

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Remark: The matrix A above is called the *Vandermonde* matrix.

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- We want to find $x = \begin{bmatrix} x_0 & x_1 & \cdots & x_{n-1} \end{bmatrix}^T$ minimizing

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Definition: An $m \times n$ system $Ax = b$ is called *overdetermined* if $m > n$.

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- Overdetermined systems are usually inconsistent. (*e.g.* It is unlikely that three lines in $\mathbf{R}^2$ intersect each other at a common point.)

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- Overdetermined systems are usually inconsistent. (*e.g.* It is unlikely that three lines in $\mathbf{R}^2$ intersect each other at a common point.)
  Example:

$$[\,A \mid b\,] = \begin{bmatrix} 1 & -2 & -1 \\ 1 & 3 & 1 \\ 1 & 4 & 2 \end{bmatrix} \rightsquigarrow \underbrace{\begin{bmatrix} 1 & -2 & -1 \\ 0 & 5 & 2 \\ 0 & 0 & 3/5 \end{bmatrix}}_{inconsistent}$$

Least Squares, Problem Definition

Justification:

$\text{range}(A) = \text{span}\{a_1, a_2, \ldots, a_n\}$ is at most an n-dimen subspace in $\mathbb{C}^m$

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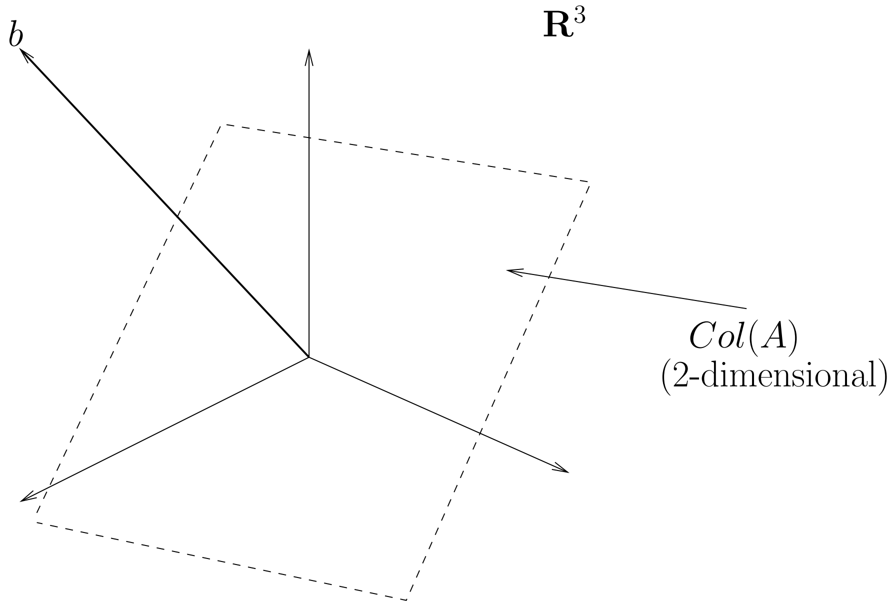

e.g. $m = 3$, $n = 2$

$$A = \begin{bmatrix} x & x \\ x & x \\ x & x \end{bmatrix}$$

Least Squares, Problem Definition

Least Squares Problem: Given an overdetermined system $Ax = b$.

Find $x \in \mathbb{C}^n$ such that $\|Ax - b\|_2$ is as small as possible.

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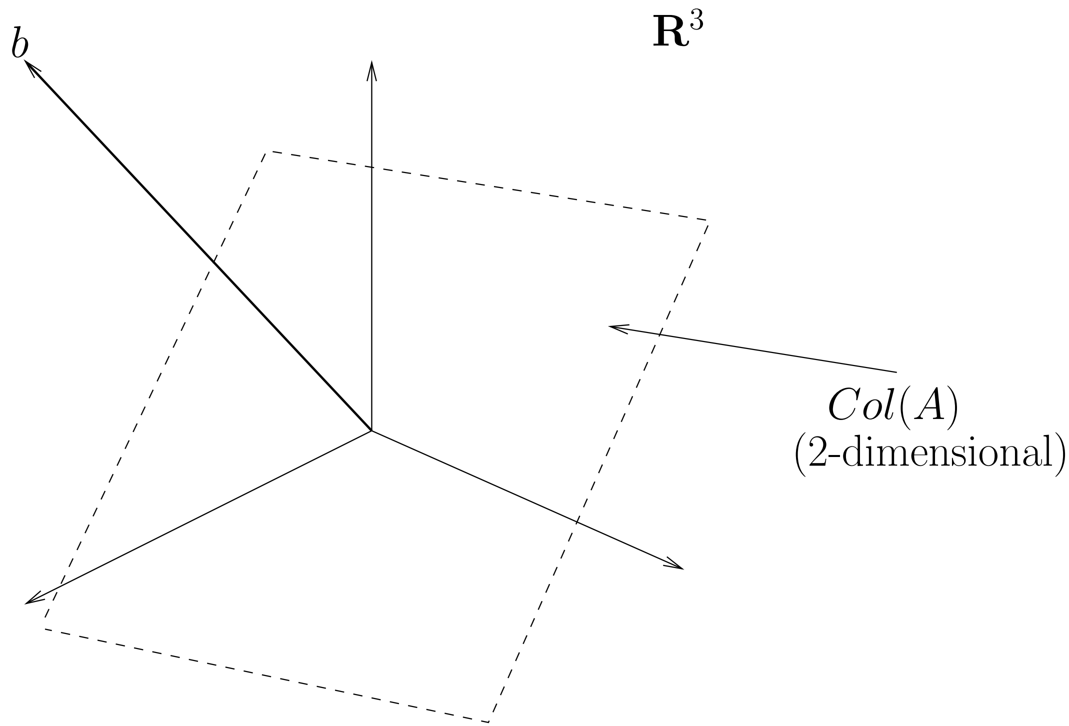
Find $x \in \mathbb{C}^n$ such that $\|Ax - b\|_2$ is as small as possible.

- Geometric interpretation: Find the point on the hyperplane $\mathrm{range}(A)$ that is closest to b.



Least Squares, Problem Definition

A motivating example

- US population as a function of time

t	y (population)
1900	75.995
1910	91.972
1920	105.711
1930	123.203
1940	131.669
1950	150.697
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- Fit a cubic model $y \approx p(t) = x_3 t^3 + x_2 t^2 + x_1 t + x_0$ approximating the US population by solving the least squares problem. Use it to estimate the US population in 2020.

Least Squares, Problem Definition

Need to find $x = \begin{bmatrix} x_0 & x_1 & x_2 & x_3 \end{bmatrix}^T \in \mathbb{R}^4$ minimizing

$$\left\| \underbrace{\begin{bmatrix} 1 & 1900 & 1900^2 & 1900^3 \\ 1 & 1910 & 1910^2 & 1910^3 \\ 1 & 1920 & 1920^2 & 1920^3 \\ 1 & 1930 & 1930^2 & 1930^3 \\ 1 & 1940 & 1940^2 & 1940^3 \\ 1 & 1950 & 1950^2 & 1950^3 \\ 1 & 1960 & 1960^2 & 1960^3 \\ 1 & 1970 & 1970^2 & 1970^3 \\ 1 & 1980 & 1980^2 & 1980^3 \\ 1 & 1990 & 1990^2 & 1990^3 \\ 1 & 2000 & 2000^2 & 2000^3 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}}_{x} - \underbrace{\begin{bmatrix} 75.995 \\ 91.972 \\ 105.711 \\ 123.203 \\ 131.669 \\ 150.697 \\ 179.323 \\ 203.212 \\ 226.505 \\ 249.633 \\ 281.422 \end{bmatrix}}_{b} \right\|$$

Least Squares, Problem Definition

The optimal cubic polynomial solving the least squares problem

$$p(t) = 56.0821 \left(\frac{t-1950}{50}\right)^3 + 127.3056 \left(\frac{t-1950}{50}\right)^2 - 80.6311 \left(\frac{t-1950}{50}\right) + 165.3947$$

Least Squares, Problem Definition

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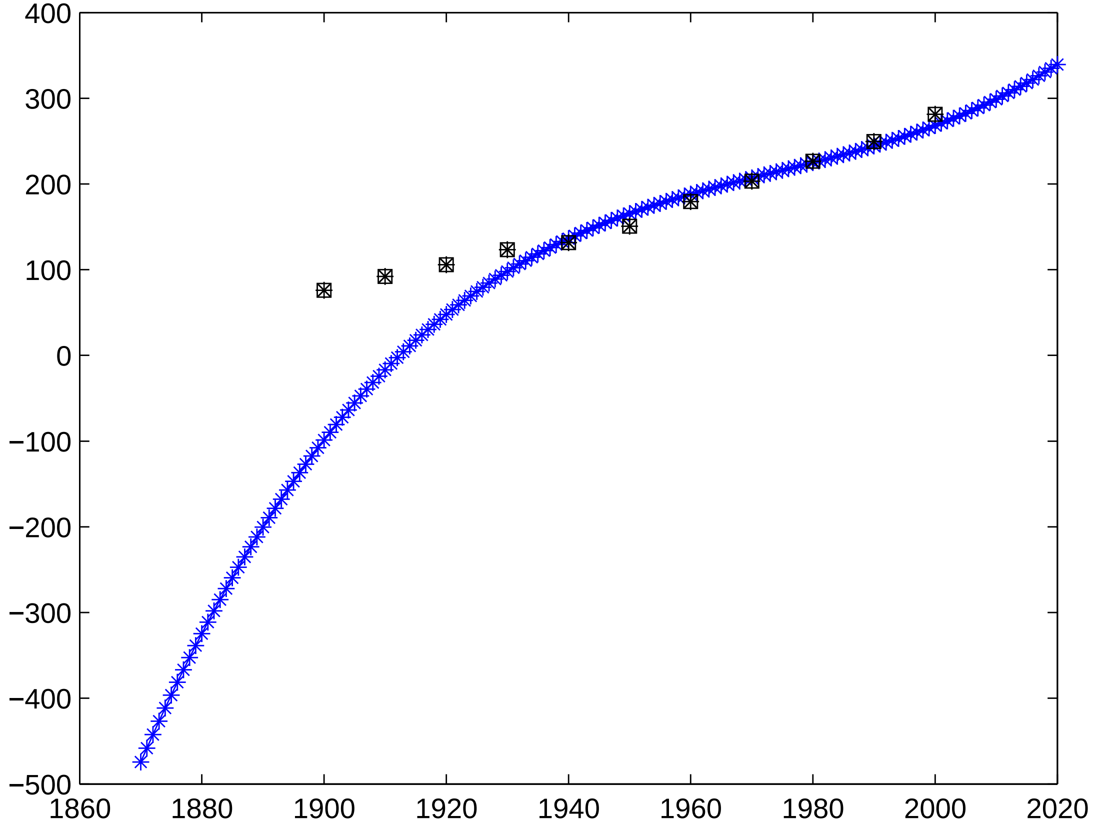

Black squares - given pairs of (year,population) data; Blue curve - optimal cubic polynomial

Next Lecture

Conditioning and condition numbers - Lecture 12