# V. Linear and Non-linear Least Squares

<u>Goals:</u> - solve overdetermined linear and nonlinear systems of equations
- linear: Normal equations and orthogonal decomposition method
- nonlinear: Newton and Gauss-Newton methods
- only the numerical aspects (statistics later...)

<u>Why:</u> - curve fitting

In practice, one often has to determine some parameters of a given function (from natural laws or model assumptions) through a series of measurements.
Usually, the number of measurements $m$ is much larger than the number of parameters $n$, that is $m \gg n$.

<u>Ex.:</u> (1) Model ① $\quad y(t) = a_1 \cdot t + a_2 \quad$ (linear)

Model ② $\quad y(t) = a_2 \cdot e^{a_1 \cdot t} \quad$ (nonlinear)

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One distinguishes:

(linear) $\quad A\vec{x} = \vec{b} \quad , A \in \mathbb{R}^{m \times n}, \vec{b} \in \mathbb{R}^m$

(nonlinear) $\quad \vec{f}(\vec{x}) = \vec{b} \quad , \vec{f} : D \subset \mathbb{R}^n \to \mathbb{R}^m$

$\vec{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$ vector of unknown parameters

However, these equations do in general not admit a solution in the common sense. Instead one looks for so-called least-squares solutions

(linear) $\quad \min\limits_{\vec{x} \in D} \| A\vec{x} - \vec{b} \|_2 = \|\vec{r}\|_2$

(nonlinear) $\quad \min\limits_{\vec{x} \in D} \| \vec{f}(\vec{x}) - \vec{b} \|_2 = \|\vec{r}\|_2$

where $\quad D$ ... admissible parameter domain

$\quad \|\_\|_2$ ... Euclidean norm $\quad \|\vec{x}\|_2 = \sqrt{x_1^2 + \ldots + x_n^2}$

$\quad = \sqrt{\vec{x}^T \vec{x}}$ transpose

$\quad \|\vec{r}\|_2$ ... residual

So one minimizes the deviation

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## V.1 Linear Least-Squares

Let's focus on the linear case:

$$\min_{\vec{x}} \phi(\vec{x})$$

where $\phi(\vec{x}) = \frac{1}{2}\|A\vec{x} - \vec{b}\|_2^2$

and $A \in \mathbb{R}^{m\times n}$, $\vec{b} \in \mathbb{R}^m$, $\vec{x} \in \mathbb{R}^n$.

Moreover, we assume that $A$ has full column rank $n$, i.e. the columns of $A$ are linearly independent.

Here as usual: $m$ ... number of measurements
$n$ ... number of parameters

<u>Rem.:</u> The assumption on the rank implies that the parameters are not ambiguous

### V.1.1 Normal equations

Let's rewrite $\phi(\vec{x})$ as:

$$\begin{aligned}
\phi(\vec{x}) &= \tfrac{1}{2}\|A\vec{x} - \vec{b}\|_2^2 \\
&= \tfrac{1}{2}(A\vec{x} - \vec{b})^T(A\vec{x} - \vec{b}) = \tfrac{1}{2}(\vec{x}^T A^T - \vec{b}^T)(A\vec{x} - \vec{b}) \\
&= \tfrac{1}{2}\Big(\vec{x}^T A^T A\vec{x} - \vec{x}^T A^T \vec{b} - \underbrace{\vec{b}^T A\vec{x}}_{=(\vec{b}^T A\vec{x})^T = \vec{x}^T A^T \vec{b}} + \vec{b}^T\vec{b}\Big)
\end{aligned}$$

scalar!

$$= \tfrac{1}{2}\left(\vec{x}^T A^T A\vec{x} - 2\vec{x}^T A^T \vec{b} + \vec{b}^T\vec{b}\right)$$

$$\left[ \sim \frac{1}{2}(x\,a\,a\,x - 2\,x\,a\,b + b\,b) = \frac{1}{2}(a^2x^2 - 2abx + b^2) \right]$$

At an extremum:

$$\vec{\nabla}\phi(\vec{x}) = A^T A \vec{x} - A^T \vec{b} \overset{!}{=} 0$$

These are the so-called normal equations and their solution is the seeked least-squares solution

Rem.: (i) The solution to the normal equations is indeed a minimum of $\phi(\vec{x})$ and it is unique:

① $A^T A$ is a positive definit matrix

$$\|A\vec{x}\|_2^2 = \underbrace{\vec{x}^T A^T A \vec{x} > 0}_{\text{Def. of positive definite}} \quad \text{for all } x \in \mathbb{R}^n, \vec{x} \neq 0$$

② $\vec{x}^T A^T A \vec{x} = 0 \iff \vec{x} = 0$

"$\Leftarrow$": clear

"$\Rightarrow$": $\underbrace{\vec{x}^T A^T}_{(A\vec{x})^T} \underbrace{A\vec{x}}_{} = 0$

$= 0 \iff \vec{x}$ because $\operatorname{rank}(A) = n$ !

✓.

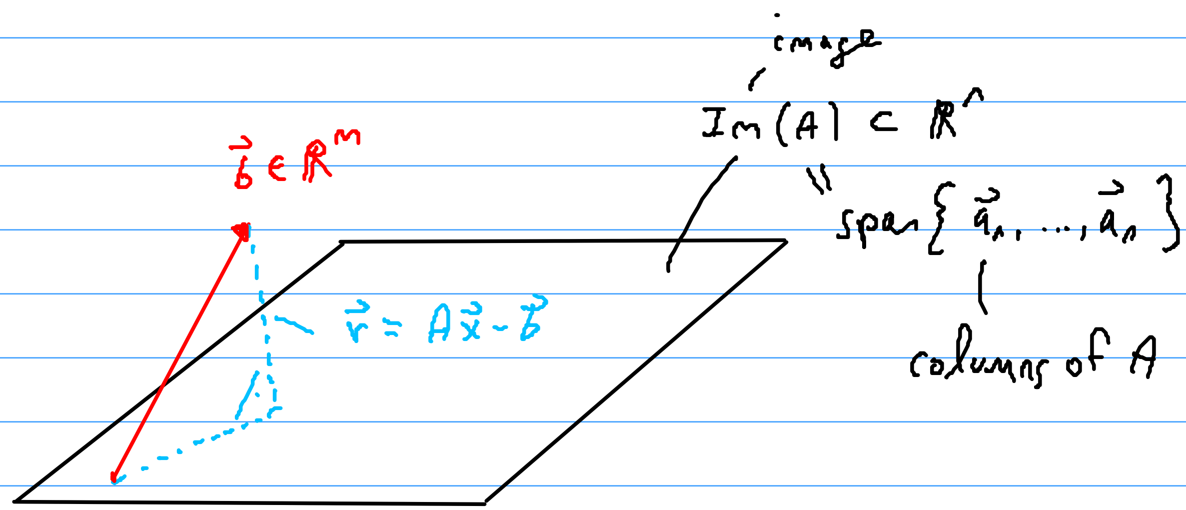
This is just a generalization of the well known fact $\frac{1}{2}(a\,a\,x^2 - 2abx + b^2) \ldots a \cdot a > 0$ for a minimum!

(ii) $A^T A \vec{x} = A^T \vec{b}$:

$$\underbrace{\left( \underset{n \times m}{A^T} \right) \left( \underset{m \times n}{A} \right)}_{\left( \underset{n \times n}{A^T A} \right)} \left( \underset{n \times 1}{\vec{x}} \right) = \underbrace{\left( \underset{n \times m}{A^T} \right) \left( \underset{m \times 1}{\vec{b}} \right)}_{\left( \underset{n \times 1}{A^T b} \right)}$$

$$\left( \underset{n \times n}{A^T A} \right) \left( \underset{n \times 1}{\vec{x}} \right) = \left( \underset{n \times 1}{A^T b} \right)$$

(iii) Geometric interpretation




minimize $\|A\vec{x} - \vec{b}\|_2 \rightsquigarrow A\vec{x} - \vec{b}$ is normal to $\mathrm{Im}(A)$

(Hence normal equations)

<u>Ex.:</u> (2) Linear model $\rightsquigarrow$ slides

However, it turns out that solving the normal equations can be problematic, i.e. ill-conditioned

(a small change in $\vec{b}$ can lead to a large change in $\vec{x}$)

Therefore the (following) orthogonal decomposition method is preferred

## V.1.2 The orthogonal decomposition method

Def.: an orthogonal matrix $Q$ is a real square matrix whose columns are orthonormal:

$$Q^T Q = Q Q^T = I = \begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}$$

Rem.: - $Q^{-1} = Q^T$

An important property of orthogonal matrices is that they don't change the Euclidean norm (i.e. length):

$$\| Q \vec{x} \|_2^2 = \vec{x}^T \underbrace{Q^T Q}_{I} \vec{x} = \vec{x}^T \vec{x} = \| \vec{x} \|_2^2$$

Fact: every matrix $A \in \mathbb{R}^{m \times n}$ with full column rank $n$ (linearly independent columns) has a so-called QR-decomposition

$$A = QR$$

where $Q \in \mathbb{R}^{m \times m}$ is an orthogonal matrix and $R \in \mathbb{R}^{m \times n}$ an upper triangular matrix with $r_{ii} \neq 0$ $(i = 1, \dots, n)$

$$\begin{pmatrix} A \\ m\times n \end{pmatrix} = \begin{pmatrix} Q \\ m\times m \end{pmatrix} \overset{R}{\begin{pmatrix} r_{11} & r_{12} & \cdots & \\ & r_{22} & & \\ 0 & & \ddots & \\ & & & r_{nn} \\ \hline & 0 & & \end{pmatrix}}$$

$$\begin{pmatrix} \overset{\text{upper triangular}}{R_1} \\ n\times n \\ \hline 0 \end{pmatrix}$$

<u>MATLAB:</u> $[Q, R] = qr(A)$

With this: Let $A = QR$

$$\|A\vec{x} - \vec{b}\|_2^2 = \|\vec{r}\|_2^2$$

(Q ortho.!) $$\|Q^T(A\vec{x} - \vec{b})\|_2^2 = \|Q^T\vec{r}\|_2^2 = \|\vec{r}\|_2^2$$

$$\|Q^T(QR\vec{x} - \vec{b})\|_2^2 = \|\vec{r}\|_2^2$$

$$\|R\vec{x} - Q^T\vec{b}\|_2^2 = \|\vec{r}\|_2^2$$

$$\left\|\begin{pmatrix} R_1 \\ \hline 0 \end{pmatrix}\vec{x} - \overset{\text{split}}{\begin{pmatrix} \vec{c} \\ \hline \vec{d} \end{pmatrix}}\right\|_2^2 = \|\vec{r}\|_2^2$$

$$\underbrace{\|R_1\vec{x} - \vec{c}\|_2^2}_{} + \|\vec{d}\|_2^2 = \|\vec{r}\|_2^2$$

n equations in n unknowns $\rightsquigarrow$ $\vec{x} = R_1^{-1}\vec{c}$

invertible because $r_{ii} \neq 0$ $(i = 1, \dots, n)$

In summary: ① $A = QR$, $Q^T\vec{b} = \begin{pmatrix}\vec{c}\\ \vec{d}\end{pmatrix}$

② $\vec{x} = R_1^{-1}\vec{c}$

③ $\|\vec{r}\|_2 = \|\vec{d}\|_2$

<u>Ex.:</u> (3) Same as ex. (2) but with QR

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(Of course, we get the same result!)

(4) Same as ex. (2) & (3) but with the MATLAB all-in-one solution: $\vec{x} = A \backslash \vec{b}$

backslash operator

## V.2 Non-linear Least-Squares

Let's now consider the case of overdetermined nonlinear systems of equations

$$f_1(x_1,\dots,x_n) = b_1$$
$$f_2(x_1,\dots,x_n) = b_2$$
$$\vdots$$
$$f_m(x_1,\dots,x_n) = b_m$$

or short $\vec{f}(\vec{x}) = \vec{b}$

$\vec{f}: D \subset \mathbb{R}^n \to \mathbb{R}^m$

$\vec{b} = \begin{pmatrix} b_1 \\ \vdots \\ b_m \end{pmatrix} \in \mathbb{R}^m$

$\vec{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \in \mathbb{R}^n$

m (nonlinear) equations in n unknowns.

Usually $m \gg n$ (many more measurements than parameters!)

Least-squares solution:

$$\min_{\vec{x} \in D} \phi(\vec{x})$$

where $\phi(\vec{x}) = \frac{1}{2} \| \vec{f}(\vec{x}) - \vec{b} \|_2^2$

Let's rewrite $\phi(\vec{x})$:

$$\phi(\vec{x}) = \frac{1}{2} \| \vec{f}(\vec{x}) - \vec{b} \|_2^2$$

$$= \frac{1}{2} \sum_{i=1}^{m} \left( f_i(\vec{x}) - b_i \right)^2$$

(not sufficient ... see below)

A necessary condition for a minimum is that the gradient of $\phi$ vanishes:

$$\vec{\nabla}\phi = \begin{pmatrix} \frac{\partial \phi}{\partial x_1} \\ \vdots \\ \frac{\partial \phi}{\partial x_n} \end{pmatrix} \overset{!}{=} 0$$

Then

$$\frac{\partial \phi}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{1}{2} \sum_{i=1}^{m} \left( f_i(x_1, \dots, x_j, \dots, x_n) - b_i \right)^2 \right)$$

$$= \sum_{i=1}^{m} \left( f_i(\vec{x}) - b_i \right) \cdot \frac{\partial f_i}{\partial x_j} \overset{!}{=} 0, \quad j = 1, \dots, n$$

These are $n$ (nonlinear) equations for the $n$ unknown parameters

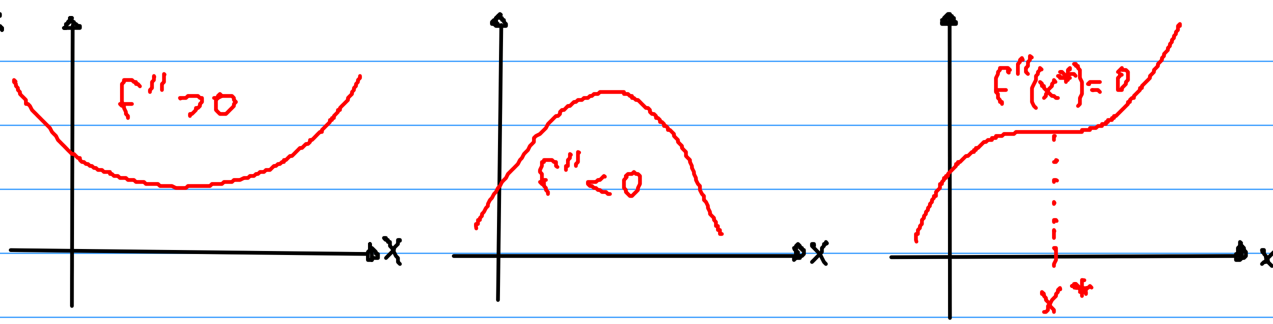
The vanishing gradient is only a necessary condition for a minimum (it could also be a maximum or a saddle point)

We need one further condition:

$$H = \underbrace{(\text{Hess}\,\phi)}_{\text{Hessian matrix}} = \left( \frac{\partial^2 \phi}{\partial x_i \, \partial x_j} \right)_{i,j} \quad \text{positiv definit}$$

i.e. $\vec{x}^T H \vec{x} > 0$ for all $\vec{x} \in \mathbb{R}^n$, $\vec{x} \neq 0$.

In one variable, this reduces to the familiar cases:



## V.2.1 Newton method

<u>Idea:</u> apply Newton's method directly to

$$\vec{\nabla}\phi \overset{!}{=} 0$$

Linearize $\vec{\nabla}\phi$ around some given $\overset{\text{k-th iteration}}{\vec{x}^{(k)}}$:

$$\vec{\nabla}\phi(\vec{x}^{(k)}) \approx \vec{\nabla}\phi(\vec{x}^{(k)}) + (\text{Hess}\,\phi)(\vec{x}^{(k)})(\vec{x} - \vec{x}^{(k)})$$

Define $\overset{\text{(k+1)-th iteration}}{\vec{x}^{(k+1)}}$ as

$$\vec{\nabla}\phi(\vec{x}^{(k)}) + (\text{Hess}\,\phi)(\vec{x}^{(k)})\underbrace{(\vec{x}^{(k+1)} - \vec{x}^{(k)})}_{\vec{s}\ \text{(call it } \vec{s}\,!)} = 0$$

Then

$$\vec{x}^{(k+1)} = \vec{x}^{(k)} + \vec{s}\ , \quad k = 0, 1, \ldots, \text{convergence}$$

$$\text{solve} \quad (\text{Hess}\,\phi)(\vec{x}^{(k)})\,\underline{\underline{\vec{s}}} = -\vec{\nabla}\phi(\vec{x}^{(k)})$$

<u>Rem.:</u> (i) if close enough to <u><u>a</u></u> minimum, it converges quadratically $p=2$ — existence & uniqueness discussion in chapter II!

(ii) needs the Hessian matrix

## V.2.2 Gauss–Newton method

Idea: linearize the residual equations $\vec{F}(\vec{x}) - \vec{b}$ and solve a sequence of linear least-squares problems

So linearize at some given $\vec{x}^{(k)}$: k-th iteration

$$\vec{F}(\vec{x}) - \vec{b} \approx \vec{F}(\vec{x}^{(k)}) - \vec{b} + J(\vec{x}^{(k)})(\vec{x} - \vec{x}^{(k)})$$

$$\rightsquigarrow \quad A^{(k)}\vec{x} - \vec{\beta}^{(k)}$$

Simply rearranging the terms... and a linear least-squares problem appears!

So instead of solving the nonlinear least-squares problem, one solves a sequence of linear least-squares problems:

$$\vec{x}^{(0)} \longrightarrow \min_{\vec{x} \in D} \frac{1}{2} \| A^{(0)}\vec{x} - \vec{\beta}^{(0)} \|_2^2 \longrightarrow \vec{x}^{(1)}$$

initial guess

$$\min_{\vec{x} \in D} \frac{1}{2} \| A^{(1)}\vec{x} - \vec{\beta}^{(1)} \|_2^2 \longrightarrow \vec{x}^{(2)}$$

$$\vdots$$

$$\min_{\vec{x} \in D} \frac{1}{2} \| A^{(k)}\vec{x} - \vec{\beta}^{(k)} \|_2^2 \longrightarrow \vec{x}^{(k+1)}$$

Stop when $\| \vec{x}^{(k+1)} - \vec{x}^{(k)} \| <$ tolerance

<u>Rem.:</u> (i) if it converges, then it converges with order $p = 1 \dots 2$

(ii) it fails if $A^{(k)}$ is very badly conditioned

$\rightsquigarrow$ Levenberg-Marquardt methods ...

<u>Ex.:</u> (5) Nonlinear least-squares $\rightsquigarrow$ Slides