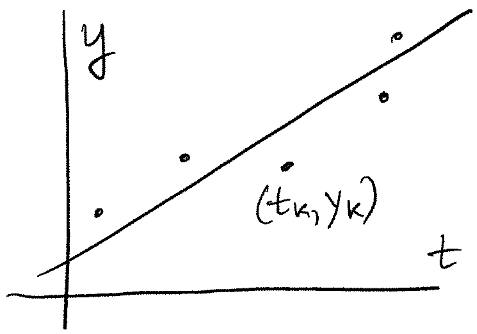
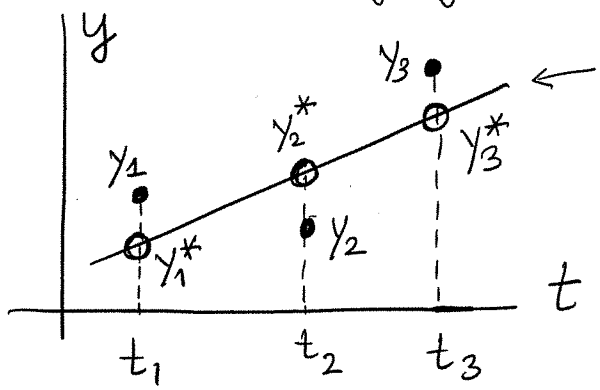
Sec. 3.8. Least squares (LS) solution to inconsistent l.s.

1 LS fit to data



Suppose we have data points that exhibit a nearly linear dependence
$y \approx a_0 + a_1 t$.
"approximately equal"

Q1: How can we find a_0, a_1 such that this straight line is the best fit to the data points?
Q2: What is "the best fit"?
We answer Q2 first, considering just three points not lying on the same line.



$y_{best}(t) = a_0 + a_1 t$.

Let $y_k^* = y_{best}(t_k)$, so that y_1^*, y_2^*, y_3^* do lie on the same line.

We call this line the best (linear) fit if:

$$\boxed{\sum_{k=1}^{\#\text{ of points}} (y_k - y_k^*)^2 = \min} \qquad (\star)$$

Since it makes the sum of **squares** of the deviations **the least**, it is called the **Least Squares (LS) fit**.

② LS approximation to the data and LS sol'n of an inconsistent l.s.

Ex. 1 Find the best (= LS) linear fit to 3 points: (t_1, y_1), (t_2, y_2), (t_3, y_3).

Sol'n: 1) seek $y_{best} = a_0 + a_1 t$, where a_0, a_1 are to be found.

@ (t_1, y_1): $a_0 \cdot 1 + a_1 \cdot t_1$ "=" y_1

@ (t_2, y_2): $a_0 \cdot 1 + a_1 \cdot t_2$ "=" y_2

@ (t_3, y_3): $a_0 \cdot 1 + a_1 \cdot t_3$ "=" y_3

Note: We wrote "=", not =, because we cannot expect that all three points will fall on the same line. So, "=" means 'approximates', not 'strictly equals'.

The previous system in matrix form is:

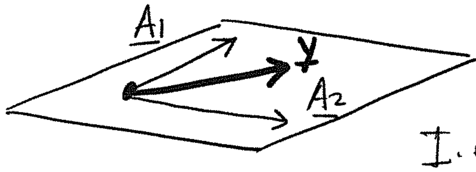
$$\Big[\underbrace{\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}}_{\underline{A_1}}, \underbrace{\begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix}}_{\underline{A_2}}\Big] \underbrace{\begin{pmatrix} a_0 \\ a_1 \end{pmatrix}}_{\substack{\underline{x} \\ \nearrow \\ \text{unknown}}} \text{"="} \underbrace{\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}}_{\underline{y}}, \quad \Rightarrow$$

$$[\underline{A_1}, \underline{A_2}] \cdot \underline{x} \text{ "=" } \underline{y} \iff A\,\underline{x} \text{ "=" } \underline{y}.$$

Using the key formula, we can also write it as:

$$x_1 \underline{A_1} + x_2 \underline{A_2} \text{ "=" } \underline{y}. \qquad (*)$$

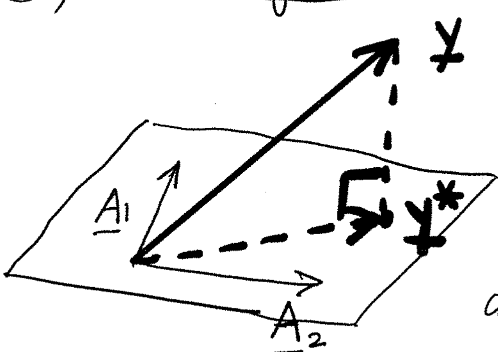
The are two possibilities with respect to the above equation:

(a) 

$\underline{y}$ lies in the plane made by $\underline{A_1}$ & $\underline{A_2}$. I.e., it is in $Sp(\{\underline{A_1}, \underline{A_2}\})$,

$\Rightarrow$ equation **(*)** on p. 16-2 is consistent. We know how to solve it (use REF). But, this situation is special, not generic; it would imply that the 3 pts in the original problem happen to be on the same straight line.

(b) The <u>generic</u> case is when $\underline{y}$ is **not** in the plane made by $\underline{A_1}$ and $\underline{A_2}$. Then $\underline{y}$ is not in $Sp(\{\underline{A_1}, \underline{A_2}\})$, and l.s. **(*)** is inconsistent.

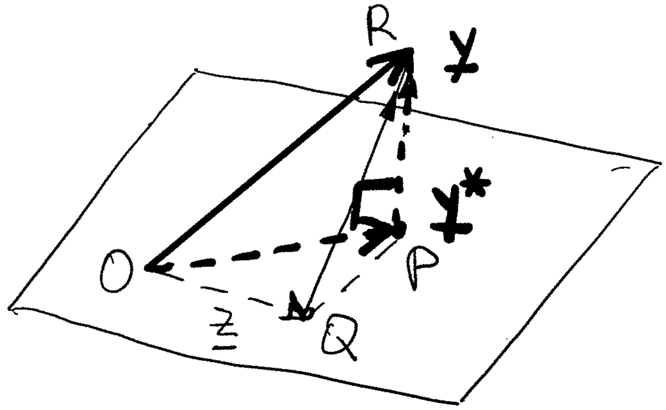


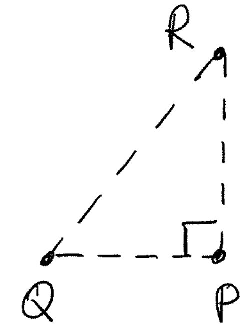
Then, instead of solving it, which is <u>impossible</u>, we will do the <u>next best thing</u>, which is <u>possible</u>: solve

$$x_1 \underline{A_1} + x_2 \underline{A_2} = \underline{y}^*, \quad (**)$$

where $\underline{y}^*$ is the projection of $\underline{y}$ on the plane made by $(\underline{A_1}, \underline{A_2})$ (i.e., $\underline{y}^*$ is in $Sp(\{\underline{A_1}, \underline{A_2}\})$).

- **Why is this y^* the <u>best</u> approximation to $\underline{y}$?**





Consider <u>any other</u> vector $\underline{z}$ in the same plane.

Note that: $\quad \vec{PR} = \underline{y} - \underline{y}^*$

$\qquad\qquad\quad \vec{QR} = \underline{y} - \underline{z}$.

Then: $\|\vec{PR}\|$ = distance between $\underline{y}$ and $\underline{y}^*$,

$\qquad\quad \|\vec{QR}\|$ = distance between $\underline{y}$ and $\underline{z}$.

Now look at the ΔRPQ in the right figure above. The angle $\angle P = 90^\circ$ because $\vec{PR} \perp$ plane and hence $\vec{PR} \perp$ any line in this plane.

From this right ΔRPQ, it is clear that $\|\vec{PR}\| < \|\vec{QR}\|$, so distance from $\underline{y}$ is the shortest to $\underline{y}^*$ among all vectors $\underline{z}$ in that plane.

Note 1: We have shown that

$$\|\vec{PR}\| \equiv \|\underline{y} - \underline{y}^*\| = \min.$$

However, $\underline{y} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$, $\underline{y}^* = \begin{pmatrix} y_1^* \\ y_2^* \\ y_3^* \end{pmatrix}$, where y_k^* are the values marked with "o" in figure on p. 16-1. (Since all y_k^* lie on the same line, the l.s. $A\underline{x} = \underline{y}^*$ is consistent, as we've seen above from another perspective.)

But then $\sum_{k=1}^{3} (y_k - y_k^*)^2 = \|\underline{y} - \underline{y}^*\|^2 = \min$, which agrees with formula (A) on p. 16-1 and justifies name 'LS'.

Note 2: Vector $\underline{y}^*$ is called the **LS approximation to the data** (i.e., to $\underline{y}$).

We will now use $\underline{y}^*$ to find $\underline{x}$, **the LS solution** to the consistent l.s. $A\underline{x} = \underline{y}^*$.

So, we need to find $\underline{y}^*$. Recall:

- $\vec{PR} = \underline{y} - \underline{y}^*$
- $\vec{PR} \perp$ plane made by $\underline{A_1}, \underline{A_2}$; $\Rightarrow \vec{PR} \perp \underline{A_1}, \underline{A_2}$.

Write this using linear algebra:

$$\begin{cases} \underline{A_1}^T(\underline{y}-\underline{y}^*) = 0 \\ \underline{A_2}^T(\underline{y}-\underline{y}^*) = 0 \end{cases} \Rightarrow \begin{bmatrix} \underline{A_1}^T \\ \underline{A_2}^T \end{bmatrix} (\underline{y}-\underline{y}^*) = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow$$

$$A^T \cdot (\underline{y} - \underline{y}^*) = \underline{\theta} \Rightarrow \boxed{A^T\underline{y} = A^T\underline{y}^*}$$

Unfortunately, this gives us $A^T\underline{y}^*$, not $\underline{y}^*$ (and remember that you cannot cancel A^T on both sides of the above equation).

So, we proceed as follows:

$$A^T(A\underline{x} = \underline{y}^*) \Rightarrow A^T(A\underline{x}) = A^T\underline{y}^* = A^T\underline{y}$$

$$\Rightarrow \boxed{(A^TA)\,\underline{x} = A^T\underline{y}}$$

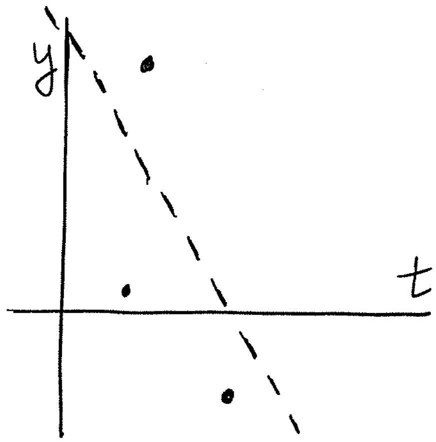
The Normal equation

The LS solution to the inconsistent l.s. $A\underline{x}$ "=" $\underline{y}$.

Ex. 2 (= Ex. 1 with numbers)

Find the best (= LS) linear fit through:

$(4,-2), (2,6), (3/2, 1/2)$.



Sol'n: 0) Seeking

$$y_{best} = a_0 + a_1 t \leftarrow \text{linear}$$

1) Setup:

$@\,(4,-2)$: $a_0 \cdot 1 + a_1 \cdot 4 \text{ "=" } -2$

$@\,(2,6)$: $a_0 \cdot 1 + a_1 \cdot 2 \text{ "=" } 6$

$@\,(\frac{3}{2}, \frac{1}{2})$: $a_0 \cdot 1 + a_1 \cdot \frac{3}{2} \text{ "=" } \frac{1}{2}$

Matrix form: $$\underbrace{\begin{pmatrix} 1 & 4 \\ 1 & 2 \\ 1 & 3/2 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} a_0 \\ a_1 \end{pmatrix}}_{\underline{x}} \text{ "=" } \underbrace{\begin{pmatrix} -2 \\ 6 \\ 1/2 \end{pmatrix}}_{\underline{y}}$$

2) Compute the ingredients of the Normal Equation:

$$A^T A = \begin{pmatrix} 1 & 1 & 1 \\ 4 & 2 & 3/2 \end{pmatrix} \begin{pmatrix} 1 & 4 \\ 1 & 2 \\ 1 & 3/2 \end{pmatrix} = \begin{pmatrix} 3 & 15/2 \\ 15/2 & 89/4 \end{pmatrix}$$

$$A^T \underline{y} = \begin{pmatrix} 1 & 1 & 1 \\ 4 & 2 & 3/2 \end{pmatrix} \begin{pmatrix} -2 \\ 6 \\ 1/2 \end{pmatrix} = \begin{pmatrix} 9/2 \\ 19/4 \end{pmatrix}$$

3) Solve the Normal Equation $(A^T A)\underline{x} = A^T \underline{y}$:

$$\begin{pmatrix} 3 & 15/2 \\ 15/2 & 89/4 \end{pmatrix} \underline{x} = \begin{pmatrix} 9/2 \\ 19/4 \end{pmatrix} \xrightarrow[\text{REF}]{} \underline{x} \equiv \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} 43/7 \\ -13/7 \end{pmatrix}.$$

Answer:

$$y_{best} = \frac{43}{7} - \frac{13}{7} t \; \underbrace{(\approx 6 - 2t)}_{\text{Needed only for the Caveat described later.}}$$

③ Discussion

Generalization 1 Exactly the same approach can be used to find LS polynomial fits (e.g., quadratic): $y_{best} = a_0 + a_1 t + a_2 t^2$.

MUST SEE Ex. 4 in textbook.

Generalization 2 Exactly the same approach can be used if instead of a linear combination of t^n (i.e., a polynomial), we use any other set of functions for a LS fit.

Ex. 3 Approximation of a function by sines and cosines (a **Fourier** series)

seek

$$y_{best} = a_0 + a_1 \cos t + a_2 \sin t + a_3 \cos 2t + a_4 \sin 2t$$

to fit through points $(t_1, y_1), \dots (t_m, y_m)$.

Follow exactly the same approach as in Ex. 1:

$$@\,(t_1, y_1):\quad a_0 \cdot 1 + a_1 \cdot \cos t_1 + a_2 \sin t_1 + a_3 \cos 2t_1 + a_4 \sin 2t_1 \;\text{"="}\; y_1$$

$$\vdots \qquad \vdots \qquad\qquad\qquad\qquad \vdots$$

$$@\,(t_m, y_m):\quad a_0 \cdot 1 + a_1 \cdot \cos t_m + a_2 \sin t_m + a_3 \cos 2t_m + a_4 \sin 2t_m \;\text{"="}\; y_m$$

In matrix form:

$$\underbrace{\begin{pmatrix} 1 & \cos t_1 & \sin t_1 & \cos 2t_1 & \sin 2t_1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \cos t_m & \sin t_m & \cos 2t_m & \sin 2t_m \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}}_{\underline{x}} \;\text{"="}\; \underbrace{\begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}}_{\underline{y}}$$

Solve the normal equation $(A^T A)\underline{x} = A^T \underline{y}$. //

Caveat Let us revisit Ex. 2.

In setting up the 3rd equation there, we had fractions 3/2 and 1/2. Since most of us do not like fractions, we can multiply that equation by 2. Then:

$$\begin{aligned} 1\cdot a_0 + 4a_1 &\text{"="} -2 \\ 1\cdot a_0 + 2a_1 &\text{"="}\ 6 \\ 2\cdot a_0 + 3a_1 &\text{"="}\ 1 \end{aligned} \Rightarrow \underbrace{\begin{pmatrix} 1 & 4 \\ 1 & 2 \\ 2 & 3 \end{pmatrix}}_{A_{new}} \underline{x} \text{ "="} \underbrace{\begin{pmatrix} -2 \\ 6 \\ 1 \end{pmatrix}}_{Y_{new}} \Rightarrow$$

solve the new Normal Eq. $\underbrace{A_{new}^T A_{new}}_{\begin{pmatrix} 6 & 12 \\ 12 & 29 \end{pmatrix}} \cdot \underline{x} = \underbrace{A_{new}^T Y_{new}}_{\begin{pmatrix} 6 \\ 7 \end{pmatrix}}$.

$\Rightarrow \underline{x} = \begin{pmatrix} 3 \\ -1 \end{pmatrix} \Rightarrow$

$(y_{best})_{new} = 3 - t$. Compare this with:

$(y_{best})_{Ex.2} \approx 6 - 2t$. They are very different!

[1] How come ?? [2] And, which one is "correct"?

Resolution: Note that in Ex. 2, we solved a problem equivalent to minimizing this sum of squares:

$$((a_0 + a_1 4) - (-2))^2 + ((a_0 + a_1 \cdot 2) - 6)^2 + ((a_0 + a_1 \cdot \tfrac{3}{2}) - \tfrac{1}{2})^2 = \min.$$

However, on this page we minimized a **different** sum:

$$\boxed{\text{same term}} + \boxed{\text{same term}} + \underbrace{\mathbf{(2a_0 + 3a_1 - 1)^2}} = \min$$

We weighed this term $\rightarrow$ **!** $4(a_0 + \tfrac{3}{2}a_1 - \tfrac{1}{2})^2$ much heavier than in Ex. 2, and 4 times heavier than the other two terms.

I.e., our new LS will have to pass much closer to point 3 than to points 1 & 2. This contradicts our original intention to treat all points equally.

Moral: When setting up a LS inconsistent l.s., do NOT multiply any equation by anything except "-1".