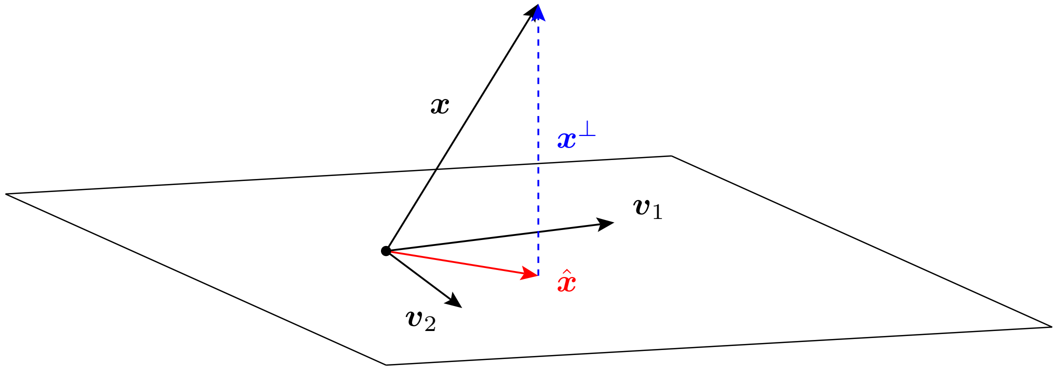
## Review

Let $W$ be a subspace of $\mathbb{R}^n$, and $\boldsymbol{x}$ in $\mathbb{R}^n$ (but maybe not in $W$).




Let $\hat{\boldsymbol{x}}$ be the **orthogonal projection** of $\boldsymbol{x}$ onto $W$.

(vector in $W$ as close as possible to $\boldsymbol{x}$)

- If $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m$ is an orthogonal basis of $W$, then

$$\hat{\boldsymbol{x}} = \underbrace{\left(\frac{\boldsymbol{x}\cdot\boldsymbol{v}_1}{\boldsymbol{v}_1\cdot\boldsymbol{v}_1}\right)\boldsymbol{v}_1}_{\text{proj. of } \boldsymbol{x} \text{ onto } \boldsymbol{v}_1} + \ldots + \underbrace{\left(\frac{\boldsymbol{x}\cdot\boldsymbol{v}_m}{\boldsymbol{v}_m\cdot\boldsymbol{v}_m}\right)\boldsymbol{v}_m}_{\text{proj. of } \boldsymbol{x} \text{ onto } \boldsymbol{v}_m}.$$

- The decomposition $\boldsymbol{x} = \underbrace{\hat{\boldsymbol{x}}}_{\text{in } W} + \underbrace{\boldsymbol{x}^\perp}_{\text{in } W^\perp}$ is unique.

## Least squares

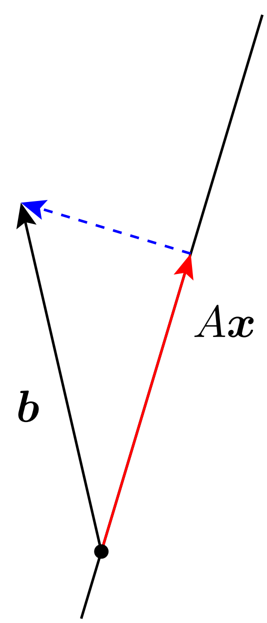
**Definition 1.** $\hat{\boldsymbol{x}}$ is a **least squares solution** of the system $A\boldsymbol{x} = \boldsymbol{b}$ if $\hat{\boldsymbol{x}}$ is such that $A\hat{\boldsymbol{x}} - \boldsymbol{b}$ is as small as possible.

- If $A\boldsymbol{x} = \boldsymbol{b}$ is consistent, then a least squares solution $\hat{\boldsymbol{x}}$ is just an ordinary solution.

  (in that case, $A\hat{\boldsymbol{x}} - \boldsymbol{b} = \boldsymbol{0}$)

- Interesting case: $A\boldsymbol{x} = \boldsymbol{b}$ is inconsistent.

  (in other words: the system is overdetermined)




**Idea.** $A\boldsymbol{x} = \boldsymbol{b}$ is consistent $\Longleftrightarrow$ $\boldsymbol{b}$ is in $\operatorname{Col}(A)$

So, if $A\boldsymbol{x} = \boldsymbol{b}$ is inconsistent, we

- replace $\boldsymbol{b}$ with its projection $\hat{\boldsymbol{b}}$ onto $\operatorname{Col}(A)$,
- and solve $A\hat{\boldsymbol{x}} = \hat{\boldsymbol{b}}$. (consistent by construction!)

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**Example 2.** Find the least squares solution to $A\boldsymbol{x} = \boldsymbol{b}$, where

$$A = \begin{bmatrix} 1 & 1 \\ -1 & 1 \\ 0 & 0 \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix}.$$

**Solution.** Note that the columns of $A$ are orthogonal.

[Otherwise, we could not proceed in the same way.]

Hence, the projection $\hat{\boldsymbol{b}}$ of $\boldsymbol{b}$ onto $\operatorname{Col}(A)$ is

$$\hat{\boldsymbol{b}} = \frac{\begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}}{\begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}} \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} + \frac{\begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}}{\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} + \frac{3}{2} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}.$$

We have already solved $A\hat{\boldsymbol{x}} = \hat{\boldsymbol{b}}$ in the process: $\hat{\boldsymbol{x}} = \begin{bmatrix} 1/2 \\ 3/2 \end{bmatrix}$.

## The normal equations

The following result provides a straightforward recipe (thanks to the FTLA) to find least squares solutions for any matrix.

[The previous example was only simple because the columns of $A$ were orthogonal.]

**Theorem 3.** $\hat{\boldsymbol{x}}$ is a least squares solution of $A\boldsymbol{x} = \boldsymbol{b}$
$\iff A^T A\hat{\boldsymbol{x}} = A^T\boldsymbol{b}$ (the **normal equations**)

**Proof.**

$\hat{\boldsymbol{x}}$ is a least squares solution of $A\boldsymbol{x} = \boldsymbol{b}$

$\iff A\hat{\boldsymbol{x}} - \boldsymbol{b}$ is as small as possible

$\iff A\hat{\boldsymbol{x}} - \boldsymbol{b}$ is orthogonal to $\operatorname{Col}(A)$

$\overset{\text{FTLA}}{\iff} A\hat{\boldsymbol{x}} - \boldsymbol{b}$ is in $\operatorname{Nul}(A^T)$

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

$\iff A^T A\hat{\boldsymbol{x}} = A^T\boldsymbol{b}$ $\square$

**Example 4. (again)** Find the least squares solution to $A\boldsymbol{x} = \boldsymbol{b}$, where

$$A = \begin{bmatrix} 1 & 1 \\ -1 & 1 \\ 0 & 0 \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix}.$$

**Solution.**

$$A^T A = \begin{bmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ -1 & 1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

$$A^T \boldsymbol{b} = \begin{bmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$$

The normal equations $A^T A \hat{\boldsymbol{x}} = A^T \boldsymbol{b}$ are

$$\begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \hat{\boldsymbol{x}} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}.$$

Solving, we find (again) $\hat{\boldsymbol{x}} = \begin{bmatrix} 1/2 \\ 3/2 \end{bmatrix}$.

**Example 5.** Find the least squares solution to $A\boldsymbol{x} = \boldsymbol{b}$, where

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

What is the projection of $\boldsymbol{b}$ onto $\mathrm{Col}(A)$?

**Solution.**

$$A^T A = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix}$$

$$A^T \boldsymbol{b} = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

The normal equations $A^T A \hat{\boldsymbol{x}} = A^T \boldsymbol{b}$ are

$$\begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix} \hat{\boldsymbol{x}} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}.$$

Solving, we find $\hat{\boldsymbol{x}} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$.

The projection of $\boldsymbol{b}$ onto $\mathrm{Col}(A)$ is $A\hat{\boldsymbol{x}} = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 4 \\ 4 \\ 3 \end{bmatrix}$.

Just to make sure: why is $A\hat{\boldsymbol{x}}$ the projection of $\boldsymbol{b}$ onto $\mathrm{Col}(A)$?

Because, for a least squares solution $\hat{\boldsymbol{x}}$, $A\hat{\boldsymbol{x}} - \boldsymbol{b}$ is as small as possible.

The projection $\hat{\boldsymbol{b}}$ of $\boldsymbol{b}$ onto $\mathrm{Col}(A)$ is

$$\hat{\boldsymbol{b}} = A\hat{\boldsymbol{x}}, \quad \text{with } \hat{\boldsymbol{x}} \text{ such that } A^T A\hat{\boldsymbol{x}} = A^T\boldsymbol{b}.$$

If $A$ has full column rank, this is (columns of $A$ independent)

$$\hat{\boldsymbol{b}} = A(A^TA)^{-1}A^T\boldsymbol{b}.$$

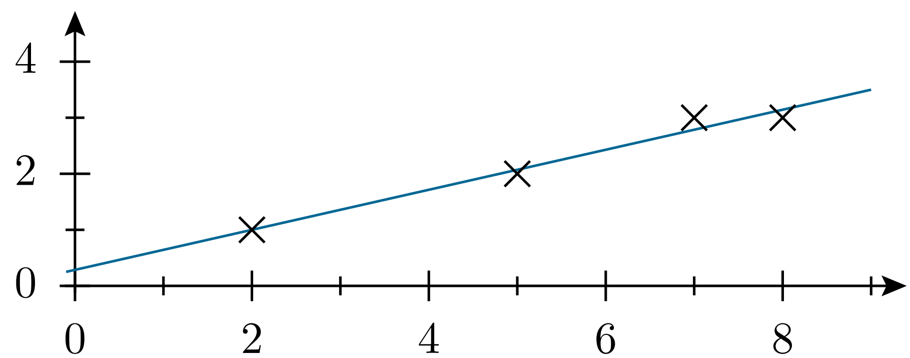
Hence, the projection matrix for projecting onto $\mathrm{Col}(A)$ is

$$P = A(A^TA)^{-1}A^T.$$

## Application: least squares lines

Experimental data: $(x_i, y_i)$

Wanted: parameters $\beta_1, \beta_2$ such that $y_i \approx \beta_1 + \beta_2 x_i$ for all $i$




This approximation should be so that

$$\underbrace{\mathrm{SS_{res}} = \sum_i [y_i - (\beta_1 + \beta_2 x_i)]^2}_{\text{residual sum of squares}} \text{ is as small as possible.}$$

**Example 6.** Find $\beta_1, \beta_2$ such that the line $y = \beta_1 + \beta_2 x$ best fits the data points $(2,1)$, $(5,2), (7,3), (8,3)$.

**Solution.** The equations $y_i = \beta_1 + \beta_2 x_i$ in matrix form:

$$\underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ 1 & x_4 \end{bmatrix}}_{\text{design matrix } X} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}}_{\text{observation vector } \boldsymbol{y}}$$

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Here, we need to find a least-squares solution to

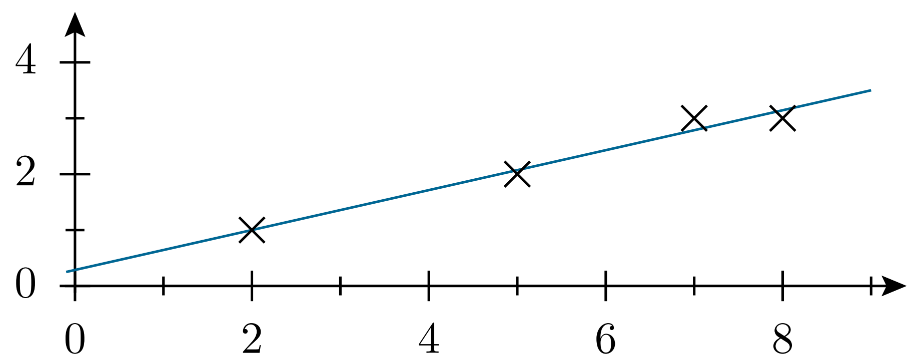
$$\begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix}.$$

$$X^T X = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix} = \begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix}$$

$$X^T \boldsymbol{y} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}$$

Solving $\begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix} \hat{\beta} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}$, we find $\begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 2/7 \\ 5/14 \end{bmatrix}$.

Hence, the least squares line is $y = \frac{2}{7} + \frac{5}{14} x$.





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