Math 415 - Lecture 24

Least squares

Wednesday October 21st 2015

Textbook reading: Chapter 3.3

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Suggested practice exercises: Exercises 3, 5, 6, 13, 24, 25

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Khan Academy video: Least Squares Approximation, Least Squares Examples, Another Least Squares Example

Review

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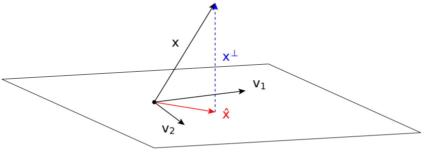

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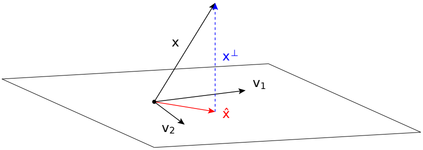

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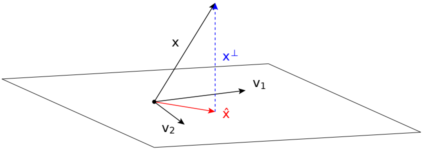

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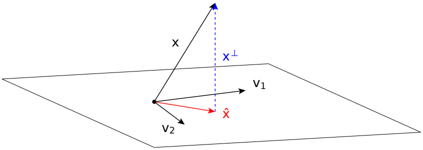

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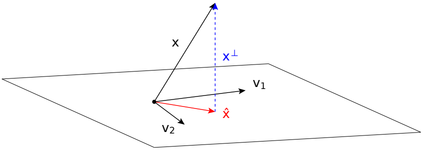

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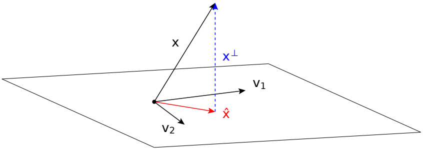

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$$\mathbf{x}_W = \underbrace{\left(\frac{\mathbf{x}\cdot\mathbf{v}_1}{\mathbf{v}_1\cdot\mathbf{v}_1}\right)\mathbf{v_1}}_{\text{proj. of } \mathbf{x} \text{ onto } \mathbf{v}_1} + \cdots + \underbrace{\left(\frac{\mathbf{x}\cdot\mathbf{v}_m}{\mathbf{v}_m\cdot\mathbf{v}_m}\right)\mathbf{v_m}}_{\text{proj. of } \mathbf{x} \text{ onto } \mathbf{v}_m}.$$

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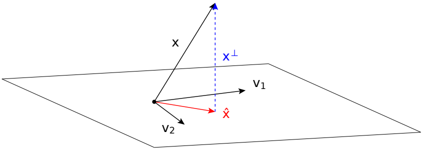

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- The decomposition $\mathbf{x} = \underbrace{\mathbf{x}_W}_{\text{in } W} + \underbrace{\mathbf{x}^\perp}_{\text{in } W^\perp}$ is unique.

Least squares

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Definition

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

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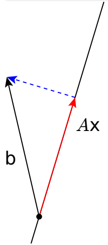

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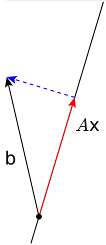

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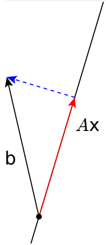

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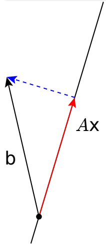

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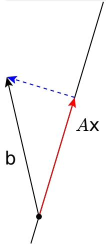

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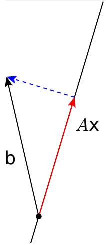

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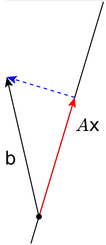

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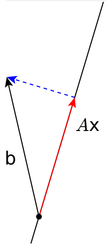

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So if $A\mathbf{x} = \mathbf{b}$ is inconsistent we

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

Example

Find the least squares solution to $A\mathbf{x} = \mathbf{b}$, where

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

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Question: What to do when the columns of A are not orthogonal?

The normal equations

Theorem

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$\hat{\mathbf{x}}$ is a least squares solution of $A\mathbf{x} = \mathbf{b}$ $\iff$ $A^T A\hat{\mathbf{x}} = A^T\mathbf{b}$

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

Example (again)

Find the least squares solution to $A\mathbf{x} = \mathbf{b}$, where

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

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

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

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

Example

Find the least squares solution to $A\mathbf{x} = \mathbf{b}$, where

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

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

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Find the least squares solution to $A\mathbf{x} = \mathbf{b}$, where

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

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Note that the columns of A are not orthogonal.

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

Applications

Least square regression lines

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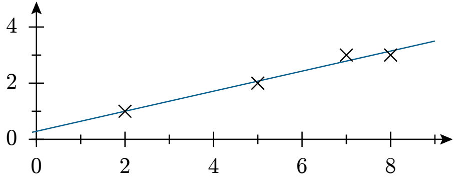

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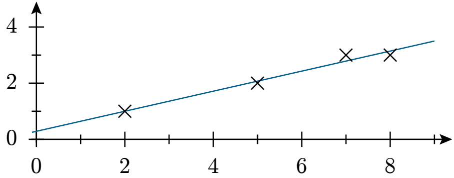

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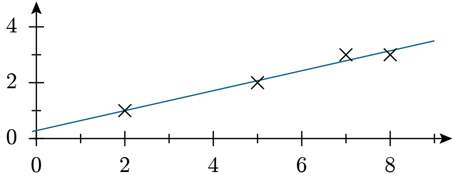

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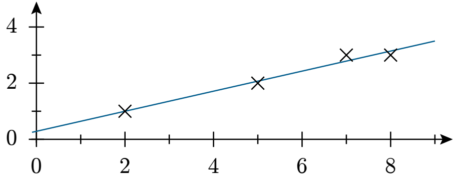

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Example

Find β_1, β_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 $y = \beta_1 + \beta_2 x$ in matrix form:

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

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Here, we need to find a least squares solution to

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

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

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Drug Dosage: D	0.0	0.2	0.4	0.6	0.8	1
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Solution

$$\underbrace{\begin{bmatrix} D_1 & 1 \\ D_2 & 1 \\ D_3 & 1 \\ D_4 & 1 \\ D_5 & 1 \\ D_6 & 1 \end{bmatrix}}_{\text{design matrix } D} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \underbrace{\begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \end{bmatrix}}_{\text{observation vector } \mathbf{c}}$$

Here, we need to find a least squares solution to $D\beta = c$ or

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Least square regression lines

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Hence the least squares line is $c = -\frac{65708}{7} d + \frac{14116}{21}$.