



NTNU
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TMA4115 - Calculus 3
Lecture 27, April 24

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Norwegian University of Science and Technology
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Review of last week's lecture



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Review of last week's lecture

Last week we introduced and studied



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- *the inner product,*



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- *the inner product,*
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- *the Gram-Schmidt process,*



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- *the Gram-Schmidt process,*
- *QR factorization.*



Today's lecture



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Today's lecture

Today we shall look at



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- *least-squares problems,*



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Today's lecture

Today we shall look at

- *least-squares problems*,
- applications to linear models.



Least-squares problems



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Least-squares problems

- Let A be an $m \times n$ matrix and \mathbf{b} a vector in \mathbb{R}^m .



Least-squares problems

- Let A be an $m \times n$ matrix and \mathbf{b} a vector in \mathbb{R}^m .
- A *least-square solution* of $A\mathbf{x} = \mathbf{b}$ is an $\hat{\mathbf{x}}$ in \mathbb{R}^n such that

$$\|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|$$

for all \mathbf{x} in \mathbb{R}^n .



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for all \mathbf{x} in \mathbb{R}^n .

- The number $\|\mathbf{b} - A\hat{\mathbf{x}}\|$ is called the *least-squares error* of $A\mathbf{x} = \mathbf{b}$.



Solution of the general least-squares problem

Theorem 13

The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ coincides with the nonempty set of solutions of the normal equation $A^T A\mathbf{x} = A^T \mathbf{b}$.



Proof of Theorem 13



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Let $\hat{\mathbf{b}} = \text{proj}_{\text{Col}(A)} \mathbf{b}$.



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Let $\hat{\mathbf{b}} = \text{proj}_{\text{Col}(A)} \mathbf{b}$. Then $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$ if and only if $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$.



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Suppose $\hat{\mathbf{x}}$ is a least-squares solutions of $A\mathbf{x} = \mathbf{b}$.



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Suppose $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$. Then $\mathbf{b} - A\hat{\mathbf{x}}$ is in $(\text{Col}(A))^\perp = \text{Nul}(A^T)$,



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Suppose $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$. Then $\mathbf{b} - \hat{\mathbf{b}} = \mathbf{b} - A\hat{\mathbf{x}}$ is in $(\text{Col}(A))^\perp = \text{Nul}(A^T)$, so $A^T(\mathbf{b} - A\hat{\mathbf{x}}) = \mathbf{0}$.



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Conversely, suppose $A^T A\hat{\mathbf{x}} = A^T \mathbf{b}$.



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Example

Let us find a least-squares solution of $A\mathbf{x} = \mathbf{b}$ where

$$A = \begin{bmatrix} 2 & 1 \\ -2 & 0 \\ 2 & 3 \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} -5 \\ 8 \\ 1 \end{bmatrix}.$$



Solution



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Solution

$$A^T A = \begin{bmatrix} 2 & -2 & 2 \\ 1 & 0 & 3 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ -2 & 0 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 4 & 8 \\ 8 & 10 \end{bmatrix}$$



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$$A^T \mathbf{b} = \begin{bmatrix} 2 & -2 & 2 \\ 1 & 0 & 3 \end{bmatrix} \begin{bmatrix} -5 \\ 8 \\ 1 \end{bmatrix} = \begin{bmatrix} -24 \\ -2 \end{bmatrix}$$



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solution of $A\mathbf{x} = \mathbf{b}$ is the same as a solution of the equation

$$\begin{bmatrix} 4 & 8 \\ 8 & 10 \end{bmatrix} \hat{\mathbf{x}} = \begin{bmatrix} -24 \\ -2 \end{bmatrix}.$$



Solution (cont.)

$$\begin{vmatrix} 4 & 8 \\ 8 & 10 \end{vmatrix} = 40 - 64 = -24,$$



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$$\begin{vmatrix} 4 & 8 \\ 8 & 10 \end{vmatrix} = 40 - 64 = -24, \text{ so } \begin{bmatrix} 4 & 8 \\ 8 & 10 \end{bmatrix} \text{ is invertible}$$



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$\begin{vmatrix} 4 & 8 \\ 8 & 10 \end{vmatrix} = 40 - 64 = -24$, so $\begin{bmatrix} 4 & 8 \\ 8 & 10 \end{bmatrix}$ is invertible and

$$\hat{\mathbf{x}} = \begin{bmatrix} 4 & 8 \\ 8 & 10 \end{bmatrix}^{-1} \begin{bmatrix} -24 \\ -2 \end{bmatrix} = \frac{1}{-24} \begin{bmatrix} 10 & -8 \\ -8 & 4 \end{bmatrix}^{-1} \begin{bmatrix} -24 \\ -2 \end{bmatrix} = \begin{bmatrix} \frac{28}{3} \\ -\frac{23}{3} \end{bmatrix} \text{ is}$$

the unique least-squares solution of $A\mathbf{x} = \mathbf{b}$.



Example

Let us find all least-squares solutions of $A\mathbf{x} = \mathbf{b}$ where

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \quad \text{and } \mathbf{b} = \begin{bmatrix} 7 \\ 2 \\ 3 \\ 6 \\ 5 \\ 4 \end{bmatrix} .$$



Solution



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Solution

$$A^T A = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 3 & 3 \\ 3 & 3 & 0 \\ 3 & 0 & 3 \end{bmatrix}$$



Solution

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$$A^T \mathbf{b} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 7 \\ 2 \\ 3 \\ 6 \\ 5 \\ 4 \end{bmatrix} = \begin{bmatrix} 27 \\ 12 \\ 15 \end{bmatrix},$$



Solution (cont.)

so a least-squares solution of $A\mathbf{x} = \mathbf{b}$ is the same as a

solution of the equation
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We reduce the augmented matrix of the above system to its reduced echelon form.



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We reduce the augmented matrix of the above system to its reduced echelon form.

$$\begin{bmatrix} 6 & 3 & 3 & 27 \\ 3 & 3 & 0 & 12 \\ 3 & 0 & 3 & 15 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{2} & \frac{9}{2} \\ 1 & 1 & 0 & 4 \\ 1 & 0 & 1 & 5 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{2} & \frac{9}{2} \\ 0 & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ 0 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix} \rightarrow$$
$$\begin{bmatrix} 1 & 0 & 1 & 5 \\ 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$



Solution

So the least-squares solutions of $A\mathbf{x} = \mathbf{b}$ are

$$\hat{\mathbf{x}} = \begin{bmatrix} 5 \\ -1 \\ 0 \end{bmatrix} + t \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix} \text{ where } t \text{ is a free parameter.}$$



Uniqueness of least-squares solutions



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Uniqueness of least-squares solutions

Theorem 14

Let A be an $m \times n$ matrix.



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- 1 The equation $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution for each \mathbf{b} in \mathbb{R}^m .



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- 1 The equation $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution for each \mathbf{b} in \mathbb{R}^m .
- 2 The columns of A are linearly independent.
- 3 The matrix $A^T A$ is invertible.

When these statements are true, the least-squares solution $\hat{\mathbf{x}}$ is given by $\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b}$.



Example

Let us find the least-squares solution of $A\mathbf{x} = \mathbf{b}$ where

$$A = \begin{bmatrix} 1 & 2 \\ -1 & 4 \\ 1 & 2 \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} 3 \\ -1 \\ 5 \end{bmatrix}.$$



Solution



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Let $\mathbf{v}_1, \mathbf{v}_2$ be the columns of A .



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Solution

Let $\mathbf{v}_1, \mathbf{v}_2$ be the columns of A . Notice that \mathbf{v}_1 and \mathbf{v}_2 are orthogonal. Recall that $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$ if and only if $A\hat{\mathbf{x}} = \text{proj}_{\text{Col}(A)} \mathbf{b}$.



Solution

Let $\mathbf{v}_1, \mathbf{v}_2$ be the columns of A . Notice that \mathbf{v}_1 and \mathbf{v}_2 are orthogonal. Recall that $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$ if and only if $A\hat{\mathbf{x}} = \text{proj}_{\text{Col}(A)} \mathbf{b}$.

$$\text{We have that } \text{proj}_{\text{Col}(A)} \mathbf{b} = \frac{\mathbf{b} \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 + \frac{\mathbf{b} \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \mathbf{v}_2 = A \begin{bmatrix} \frac{\mathbf{b} \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \\ \frac{\mathbf{b} \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \end{bmatrix},$$



Solution

Let $\mathbf{v}_1, \mathbf{v}_2$ be the columns of A . Notice that \mathbf{v}_1 and \mathbf{v}_2 are orthogonal. Recall that $\hat{\mathbf{x}}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$ if and only if $A\hat{\mathbf{x}} = \text{proj}_{\text{Col}(A)} \mathbf{b}$.

We have that $\text{proj}_{\text{Col}(A)} \mathbf{b} = \frac{\mathbf{b} \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 + \frac{\mathbf{b} \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \mathbf{v}_2 = A \begin{bmatrix} \frac{\mathbf{b} \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \\ \frac{\mathbf{b} \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \end{bmatrix}$, so

$$\hat{\mathbf{x}} = \begin{bmatrix} \frac{\mathbf{b} \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \\ \frac{\mathbf{b} \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2} \end{bmatrix} = \begin{bmatrix} 3 \\ \frac{1}{2} \end{bmatrix}.$$



QR-factorization and least-squares solutions



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QR-factorization and least-squares solutions

Theorem 15

Let A be an $m \times n$ matrix with linearly independent columns, let $A = QR$ be a QR-factorization of A and let \mathbf{b} be in \mathbb{R}^m . Then $\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b}$ is the unique least-squares solution of $A\mathbf{x} = \mathbf{b}$.



Proof of Theorem 15



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Since the columns of Q forms an orthonormal basis of $\text{Col}(A)$, it follows that $\text{proj}_{\text{Col}(A)} \mathbf{b} = QQ^T \mathbf{b}$.



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Let $\hat{\mathbf{x}} = R^{-1} Q^T \mathbf{b}$.



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Let $\hat{\mathbf{x}} = R^{-1}Q^T \mathbf{b}$. Then

$$A\hat{\mathbf{x}} = QRR^{-1}Q^T \mathbf{b} = QQ^T \mathbf{b} = \text{proj}_{\text{Col}(A)} \mathbf{b},$$



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Since the columns of Q forms an orthonormal basis of $\text{Col}(A)$, it follows that $\text{proj}_{\text{Col}(A)} \mathbf{b} = QQ^T \mathbf{b}$.

Let $\hat{\mathbf{x}} = R^{-1}Q^T \mathbf{b}$. Then

$A\hat{\mathbf{x}} = QRR^{-1}Q^T \mathbf{b} = QQ^T \mathbf{b} = \text{proj}_{\text{Col}(A)} \mathbf{b}$, so $\hat{\mathbf{x}}$ is the unique least-squares solution of $A\mathbf{x} = \mathbf{b}$.



Example

$$\text{Suppose that } A = \begin{bmatrix} 1 & -1 \\ 1 & 4 \\ 1 & -1 \\ 1 & 4 \end{bmatrix} = \begin{bmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \\ 1/2 & -1/2 \\ 1/2 & 1/2 \end{bmatrix} \begin{bmatrix} 2 & 3 \\ 0 & 5 \end{bmatrix}.$$

Let us find the least-squares solution of $A\mathbf{x} = \mathbf{b}$ where

$$\mathbf{b} = \begin{bmatrix} -1 \\ 6 \\ 5 \\ 7 \end{bmatrix}.$$



Solution



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Solution

The least-squares solution of $A\mathbf{x} = \mathbf{b}$ is

$$\begin{aligned}\hat{\mathbf{x}} &= R^{-1}Q^T\mathbf{b} = \begin{bmatrix} 2 & 3 \\ 0 & 5 \end{bmatrix}^{-1} \begin{bmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \\ 1/2 & -1/2 \\ 1/2 & 1/2 \end{bmatrix}^T \begin{bmatrix} -1 \\ 6 \\ 5 \\ 7 \end{bmatrix} \\ &= \frac{1}{10} \begin{bmatrix} 5 & -3 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{-1}{2} & \frac{1}{2} & \frac{-1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} -1 \\ 6 \\ 5 \\ 7 \end{bmatrix} \\ &= \frac{1}{20} \begin{bmatrix} 5 & -3 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 17 \\ 9 \end{bmatrix} = \frac{1}{20} \begin{bmatrix} 58 \\ 18 \end{bmatrix} = \begin{bmatrix} 2.9 \\ 0.9 \end{bmatrix}\end{aligned}$$



Least-squares lines



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Least-squares lines

- Suppose we are given a finite number of points $(x_1, y_1), \dots, (x_n, y_n)$.



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 - $\beta_0 + \beta_1 x_j$ for the *predicted* value of y ,
 - $y_j - (\beta_0 + \beta_1 x_j)$ for the *residual*.
- The *least-squares line* is the line $y = \beta_0 + \beta_1 x$ that minimizes the sum of the squares of the residuals.



Finding the least-squares line

Finding the least-squares line is equivalent to computing the least-squares solution of the equation $X\beta = \mathbf{y}$ where

$$X = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}, \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} \text{ and } \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}.$$



Example

Let us determine the equation $y = \beta_0 + \beta_1 x$ of the least-squares line that best fits the data points $(1,0)$, $(2,1)$, $(4,2)$ and $(5,3)$.



Solution

$$\text{Let } X = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 4 \\ 1 & 5 \end{bmatrix} \text{ and } \mathbf{y} = \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \end{bmatrix}.$$



Solution

$$\text{Let } X = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 4 \\ 1 & 5 \end{bmatrix} \text{ and } \mathbf{y} = \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \end{bmatrix}. \text{ Then}$$

$$X^T X = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 5 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 4 \\ 1 & 5 \end{bmatrix} = \begin{bmatrix} 4 & 12 \\ 12 & 46 \end{bmatrix} \text{ and}$$

$$X^T \mathbf{y} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 5 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 6 \\ 25 \end{bmatrix}.$$



Solution (cont.)

The columns of X are linearly independent



Solution (cont.)

The columns of X are linearly independent so the equation $X\beta = \mathbf{y}$ has a unique least-squares solution which is

$$\begin{aligned}\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} &= (X^T X)^{-1} X^T \mathbf{y} = \begin{bmatrix} 4 & 12 \\ 12 & 46 \end{bmatrix}^{-1} \begin{bmatrix} 6 \\ 25 \end{bmatrix} \\ &= \frac{1}{186 - 144} \begin{bmatrix} 46 & -12 \\ -12 & 4 \end{bmatrix} \begin{bmatrix} 6 \\ 25 \end{bmatrix} \\ &= \frac{1}{40} \begin{bmatrix} -24 \\ 28 \end{bmatrix} = \begin{bmatrix} -0.6 \\ 0.7 \end{bmatrix}\end{aligned}$$



Solution (cont.)

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so $y = -0.6 + 0.7x$ is the equation of the least-squares line that best fits the data points.



The general linear model



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The general linear model

- Any equation of the form $X\beta = \mathbf{y} + \epsilon$ where X and \mathbf{y} are given, is referred to as a *linear model*.



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The general linear model

- Any equation of the form $X\beta = \mathbf{y} + \epsilon$ where X and \mathbf{y} are given, is referred to as a *linear model*.
- The goal is to minimize the length of the *residual vector* ϵ .
- This amounts to finding a least-squares solution of $X\beta = \mathbf{y}$.



Example

Suppose data points $(x_1, y_1), \dots, (x_n, y_n)$ appear to lie along a parabola.

Suppose we wish to approximate the data by an equation of the form $y = \beta_0 + \beta_1 x + \beta_2 x^2$.

Let us describe the linear model that produces a least-square fit of the data point to the above equation.



Solution



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Solution

$$\text{Let } \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{bmatrix}, \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} \text{ and}$$

$$\boldsymbol{\epsilon} = \begin{bmatrix} y_1 - (\beta_0 + \beta_1 x_1 + \beta_2 x_1^2) \\ \vdots \\ y_n - (\beta_0 + \beta_1 x_n + \beta_2 x_n^2) \end{bmatrix}.$$



Solution

$$\text{Let } \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{bmatrix}, \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} \text{ and}$$

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Then $\mathbf{X}\boldsymbol{\beta} = \mathbf{y} + \boldsymbol{\epsilon}$ is the linear model that produces a least-square fit of the data point to the equation

$$y = \beta_0 + \beta_1 x + \beta_2 x^2.$$



Example

Suppose we are given data points $(u_1, v_1, y_1), \dots, (u_n, v_n, y_n)$ that we expect to satisfy an equation of the form

$$y = \beta_0 + \beta_1 u + \beta_2 v.$$

Let us describe the linear model that produces a least-square fit of the data point to the above equation.



Solution



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Solution

$$\text{Let } \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \mathbf{X} = \begin{bmatrix} 1 & u_1 & v_1 \\ \vdots & \vdots & \vdots \\ 1 & u_n & v_n \end{bmatrix}, \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} \text{ and}$$

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Solution

$$\text{Let } \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \mathbf{X} = \begin{bmatrix} 1 & u_1 & v_1 \\ \vdots & \vdots & \vdots \\ 1 & u_n & v_n \end{bmatrix}, \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} \text{ and}$$

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$$y = \beta_0 + \beta_1 u + \beta_2 v.$$



Tomorrow's lecture

Tomorrow we shall introduce and study

- *symmetric matrices*,
- *quadratic forms*.

Sections 7.1–7.2 in “Linear Algebras and Its Applications” (pages 393–407).

