

# Introduction to Probabilistic Machine Learning

Ralf Herbrich, Rainer Schlosser

Tutorial 7 – Recap Theory Unit 7

# Overview

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## 1. Questions and Updates

2. Recap: Unit 7, Linear Algebra, and the Inverse of a Matrix
3. Recap: Cholesky Decomposition
4. Recap: Linear Regression in Matrix Notation

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# Course Overview

Week	Topic Lecture	Tutorial	Exercises
07.04. & 08.04.	1 Probability Theory	Intro Julia	
14.04. & 15.04.	2 Inference Methods and Decision-Making	no tutorial	Exercise 1
21.04. & 22.04.	<b>no lecture</b>	Theory Unit 1 & 2	(14.04. – 08.05.)
28.04. & 29.04.	3 Graphical Models: Independence	Theory Unit 3	
05.05. & 06.05.	4 Graphical Models: Exact Inference	Theory Unit 4	Exercise 2
12.05. & 13.05.	5 Graphical Models: Approximate Inference	Theory Unit 5	(05.05. – 19.05.)
19.05. & 20.05.	6 Bayesian Ranking	Theory Unit 6	<b>Exercise 3</b>
26.05. & 27.05.	<b>7 Linear Basis Function Models</b>	<b>Theory Unit 7</b>	<b>(19.05. – 05.06.)</b>
02.06. & 03.06.	8 Bayesian Regression	Theory Unit 8	Exercise 4
09.06. & 10.06.	<b>no lecture</b>	9 Bayesian Classification	(02.06. – 23.06.)
16.06. & 17.06.	10 Non-Bayesian Classification Learning	Theory Unit 9 & 10	
23.06. & 24.06.	11 Gaussian Processes	Theory Unit 11	Exercise 5
30.06. & 01.07.	12 Information Theory	Theory Unit 12	(23.06. – 07.07.)
07.07. & 08.07.	13 Real-World Applications		

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## Recap Unit 7: Overview of Concepts and Focus

- a) Linear Basis Function Models
- b) Modelling Data (Text and Images)
- c) Linear Mappings and Matrices
- d) Singular Value Decomposition

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# Matrix-Multiplication

**Vector:** An  $n$ -dimensional vector  $\mathbf{x}$  is a column  $\vec{x} = \begin{pmatrix} x_1 \\ \dots \\ x_n \end{pmatrix}$ ,  $\vec{x}^T = (x_1 \dots x_n)$  is a row

**Matrix:** An  $n \times m$  matrix has  $n$  rows and  $m$  columns

$$\begin{pmatrix} m_{1,1} & m_{1,m} \\ m_{n,1} & m_{n,m} \end{pmatrix}$$

# Matrix-Multiplication

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**Product:** An  $n \times m$  matrix times an  $m \times k$  matrix is of ??? Format

Does the order matter? Is  $A \times B = B \times A$  ?

# Matrix-Multiplication

**Vector:** An  $n$ -dimensional vector  $\mathbf{x}$  is a column  $\vec{x} = \begin{pmatrix} x_1 \\ \dots \\ x_n \end{pmatrix}$ ,  $\vec{x}^T = (x_1 \dots x_n)$  is a row

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$$\begin{pmatrix} m_{1,1} & \dots & m_{1,m} \\ \vdots & \ddots & \vdots \\ m_{n,1} & \dots & m_{n,m} \end{pmatrix}$$

**Product:** An  $n \times m$  matrix times an  $m \times k$  matrix is of  $n \times k$  format

Examples:

$$\underbrace{(x_1 \dots x_n)}_{1 \times n} \cdot \underbrace{\begin{pmatrix} y_1 \\ \dots \\ y_n \end{pmatrix}}_{n \times 1} = \underbrace{(\dots)}_{1 \times 1} \in \mathbb{R}$$

$$\underbrace{\begin{pmatrix} x_1 \\ \dots \\ x_n \end{pmatrix}}_{n \times 1} \cdot \underbrace{(y_1 \dots y_n)}_{1 \times n} = \underbrace{\begin{pmatrix} m_{1,1} & \dots & m_{1,n} \\ \vdots & \ddots & \vdots \\ m_{n,1} & \dots & m_{n,n} \end{pmatrix}}_{n \times n} \in \mathbb{R}^{n \times n}$$



## Recap: Inverse of a Matrix

**Existence:** An  $n \times n$  matrix  $A$  is regular, i.e., has an inverse  $A^{-1}$  if, e.g.,

- $A$  has full rank
- $\det(A) \neq 0$

**Property:**  $A \cdot A^{-1} = A^{-1} \cdot A = I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dots & 0 \\ 0 & 0 & 1 \end{pmatrix}$

**Solves:**  $A \cdot \vec{x} = \vec{b} \Leftrightarrow \underbrace{A^{-1} \cdot A}_I \cdot \vec{x} = A^{-1} \cdot \vec{b}$

## To Solve $Ax=b$ : Compute the Inverse of a Matrix

**Computation 1:** Given a regular  $n \times n$  matrix  $A$ , the inverse  $A^{-1}$  can be computed as follows ??

# To Solve $Ax=b$ : Compute the Inverse of a Matrix

**Computation 1:** Given a regular  $n \times n$  matrix  $A$ , the inverse  $A^{-1}$  can be computed as follows:

$$\begin{aligned}
 & \left( \begin{array}{c|ccc} & & 1 & 0 & 0 \\ & A & 0 & \dots & 0 \\ & & 0 & 0 & 1 \end{array} \right) \\
 & \Leftrightarrow \dots \\
 & \Leftrightarrow \left( \begin{array}{c|ccc} 1 & 0 & 0 & & \\ 0 & \dots & 0 & & \\ 0 & 0 & 1 & & \end{array} \begin{array}{c} \\ A^{-1} \\ \end{array} \right)
 \end{aligned}$$

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Allowed: (i) switch rows, (ii) multiply row with nonzero scalars, (iii) add rows **11**

## To Solve $Ax=b$ : Compute the Inverse of a Matrix

**Computation 2:** Given a regular  $n \times n$  matrix  $A$ , the inverse  $A^{-1}$  can be computed as follows:

$$\begin{pmatrix} A \end{pmatrix} \cdot \begin{pmatrix} X \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dots & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Solve a **Linear Program** (LP) with ??

## To Solve $Ax=b$ : Compute the Inverse of a Matrix

**Computation 2:** Given a regular  $n \times n$  matrix  $A$ , the inverse  $A^{-1}$  can be computed as follows:

$$\begin{pmatrix} A \end{pmatrix} \cdot \begin{pmatrix} X \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dots & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Solve a **Linear Program** (LP) with  $n \times n$  variables (cf.  $X$ ) and  $n \times n$  constraints:

$$\sum_{k=1, \dots, n} A_{i,k} \cdot X_{k,j} = 1_{\{i=j\}} \quad \forall i, j = 1, \dots, n$$

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## To Solve $Ax=b$ : Compute the Inverse of a Matrix

**Computation 3:** Given a regular  $n \times n$  matrix  $A$ , the inverse  $A^{-1}$  can be computed as follows:

Use **Singular Value Decomposition** ( $U, V$  orthogonal,  $\Sigma$  diagonal):

$$A = U \cdot \Sigma \cdot V^T \quad \Leftrightarrow \quad A^{-1} = ??$$

## To Solve $Ax=b$ : Compute the Inverse of a Matrix

**Computation 3:** Given a regular  $n \times n$  matrix  $A$ , the inverse  $A^{-1}$  can be computed as follows:

Use **Singular Value Decomposition** ( $U, V$  orthogonal,  $\Sigma$  diagonal):

$$A = U \cdot \Sigma \cdot V^T \quad \Leftrightarrow \quad A^{-1} = V \cdot \Sigma^{-1} \cdot U^T$$

Note:  $V^T \cdot V = U^T \cdot U = I$

$$A \cdot A^{-1} = U \cdot \Sigma \cdot \underbrace{V^T \cdot V}_I \cdot \Sigma^{-1} \cdot U^T = I$$

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# To Solve $Ax=b$ : Cholesky Decomposition

**Computation 4:** Given a  $n \times n$  matrix  $A$  (**symmetric**, positive-semidefinite)  
we can compute a lower triangular matrix  $L$  such that:

$$L \cdot L^T = \begin{pmatrix} \cdot & 0 & 0 \\ \cdot & \cdot & 0 \\ \bullet & \cdot & \cdot \end{pmatrix} \cdot \begin{pmatrix} \cdot & \cdot & \bullet \\ 0 & \cdot & \cdot \\ 0 & 0 & \cdot \end{pmatrix} = \begin{pmatrix} & & \\ & A & \\ & & \end{pmatrix}$$

Then (Outlook): *Ansatz*:  $L \cdot \underbrace{L^T \vec{x}}_{\vec{y}} = \vec{b}$     *Then*:  $L, \vec{b} \Rightarrow \vec{y}$      $L, \vec{y} \Rightarrow \vec{x}$  (fast & stable!)

**How to get  $L$ ?** Note, again the  $\sim n \times n / 2$  constraints determine  $L$ :

$$\sum_{k=1, \dots, n} L_{i,k} \cdot L_{k,j}^T = \sum_{k=1, \dots, n} L_{i,k} \cdot L_{j,k} = A_{i,j} \quad \forall i, j = 1, \dots, n$$

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## To Solve $Ax=b$ : Cholesky Decomposition

$$\begin{aligned} \mathbf{A} = \mathbf{L}\mathbf{L}^T &= \begin{pmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{pmatrix} \begin{pmatrix} L_{11} & L_{21} & L_{31} \\ 0 & L_{22} & L_{32} \\ 0 & 0 & L_{33} \end{pmatrix} \\ &= \begin{pmatrix} L_{11}^2 & & \\ L_{21}L_{11} & L_{21}^2 + L_{22}^2 & \\ L_{31}L_{11} & L_{31}L_{21} + L_{32}L_{22} & L_{31}^2 + L_{32}^2 + L_{33}^2 \end{pmatrix} \quad (\text{symmetric}) \end{aligned}$$

# To Solve $Ax=b$ : Cholesky Decomposition

$$\begin{aligned}
 \mathbf{A} = \mathbf{L}\mathbf{L}^T &= \begin{pmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{pmatrix} \begin{pmatrix} L_{11} & L_{21} & L_{31} \\ 0 & L_{22} & L_{32} \\ 0 & 0 & L_{33} \end{pmatrix} \\
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 \end{aligned}$$

$$\sum_{k=1, \dots, n} L_{1,k} \cdot L_{1,k} = L_{1,1} \cdot L_{1,1} + 0 \cdot 0 + 0 \cdot 0 = A_{1,1}$$

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# To Solve $Ax=b$ : Cholesky Decomposition

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$$\sum_{k=1, \dots, n} L_{2,k} \cdot L_{2,k} = L_{2,1} \cdot L_{2,1} + L_{2,2} \cdot L_{2,2} + 0 \cdot 0 = A_{2,2}$$

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# To Solve $Ax=b$ : Cholesky Decomposition

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$$\sum_{k=1, \dots, n} L_{1,k} \cdot L_{1,k} = L_{1,1} \cdot L_{1,1} + 0 \cdot 0 + 0 \cdot 0 = A_{1,1} \quad \longrightarrow \quad L_{1,1} \cdot L_{1,1} = A_{1,1} \quad \Rightarrow \quad L_{1,1} = \sqrt{A_{1,1}}$$

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$$\sum_{k=1, \dots, n} L_{2,k} \cdot L_{2,k} = L_{2,1} \cdot L_{2,1} + L_{2,2} \cdot L_{2,2} + 0 \cdot 0 = A_{2,2}$$

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$$\sum_{k=1, \dots, n} L_{1,k} \cdot L_{1,k} = L_{1,1} \cdot L_{1,1} + 0 \cdot 0 + 0 \cdot 0 = A_{1,1} \quad \longrightarrow \quad L_{1,1} \cdot L_{1,1} = A_{1,1} \quad \Rightarrow \quad L_{1,1} = \sqrt{A_{1,1}}$$

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...

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# To Solve $Ax=b$ : Cholesky Decomposition

$$\begin{aligned}
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 \end{aligned}$$

$$\mathbf{L} = \begin{pmatrix} \sqrt{A_{11}} & 0 & 0 \\ A_{21}/L_{11} \xrightarrow{\text{red arrow}} \sqrt{A_{22} - L_{21}^2} & 0 & 0 \\ A_{31}/L_{11} & (A_{32} - L_{31}L_{21})/L_{22} & \sqrt{A_{33} - L_{31}^2 - L_{32}^2} \end{pmatrix}$$

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# To Solve $Ax=b$ : Cholesky Decomposition

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# To Solve $Ax=b$ : Cholesky Decomposition

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Diagram illustrating the calculation of the elements of  $\mathbf{L}$  from the elements of  $\mathbf{A}$ :

- $L_{11} = \sqrt{A_{11}}$
- $L_{21} = A_{21}/L_{11}$
- $L_{31} = A_{31}/L_{11}$
- $L_{22} = \sqrt{A_{22} - L_{21}^2}$
- $L_{32} = (A_{32} - L_{31}L_{21})/L_{22}$
- $L_{33} = \sqrt{A_{33} - L_{31}^2 - L_{32}^2}$

# To Solve $Ax=b$ : Cholesky Decomposition

$$\begin{aligned}
 \mathbf{A} = \mathbf{L}\mathbf{L}^T &= \begin{pmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{pmatrix} \begin{pmatrix} L_{11} & L_{21} & L_{31} \\ 0 & L_{22} & L_{32} \\ 0 & 0 & L_{33} \end{pmatrix} \\
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 \end{aligned}$$

General formula to compute  $L$  ??

$$\mathbf{L} = \begin{pmatrix} \sqrt{A_{11}} & 0 & 0 \\ A_{21}/L_{11} & \sqrt{A_{22} - L_{21}^2} & 0 \\ A_{31}/L_{11} & (A_{32} - L_{31}L_{21})/L_{22} & \sqrt{A_{33} - L_{31}^2 - L_{32}^2} \end{pmatrix}$$

Diagram illustrating the computation of  $L$  elements from  $A$  elements:

- $\sqrt{A_{11}}$  is the first element of  $L$ .
- $A_{21}/L_{11}$  is the second element of  $L$ .
- $A_{31}/L_{11}$  is the third element of  $L$ .
- $\sqrt{A_{22} - L_{21}^2}$  is the fourth element of  $L$ .
- $(A_{32} - L_{31}L_{21})/L_{22}$  is the fifth element of  $L$ .
- $\sqrt{A_{33} - L_{31}^2 - L_{32}^2}$  is the sixth element of  $L$ .

$$\text{Order of computation} = \begin{pmatrix} 1 \\ 2 & 3 \\ 2 & 4 & 5 \\ 2 & 6 & 7 & 8 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 1 \\ 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 & 10 \end{pmatrix}$$

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# To Solve $Ax=b$ : Cholesky Decomposition

$$\begin{aligned}
 \mathbf{A} = \mathbf{L}\mathbf{L}^T &= \begin{pmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{pmatrix} \begin{pmatrix} L_{11} & L_{21} & L_{31} \\ 0 & L_{22} & L_{32} \\ 0 & 0 & L_{33} \end{pmatrix} \\
 &= \begin{pmatrix} \boxed{L_{11}^2} & & \\ \boxed{L_{21}L_{11}} & L_{21}^2 + \boxed{L_{22}^2} & \\ \boxed{L_{31}L_{11}} & L_{31}L_{21} + \boxed{L_{32}L_{22}} & L_{31}^2 + L_{32}^2 + \boxed{L_{33}^2} \end{pmatrix} \quad (\text{symmetric})
 \end{aligned}$$

$$\mathbf{L} = \begin{pmatrix} \sqrt{A_{11}} & 0 & 0 \\ A_{21}/L_{11} & \sqrt{A_{22} - L_{21}^2} & 0 \\ A_{31}/L_{11} & (A_{32} - L_{31}L_{21})/L_{22} & \sqrt{A_{33} - L_{31}^2 - L_{32}^2} \end{pmatrix}$$

Diagram illustrating the computation of  $L$  from  $A$  using red arrows:

- $A_{11} \rightarrow \sqrt{A_{11}}$
- $A_{21} \rightarrow A_{21}/L_{11}$
- $A_{22} \rightarrow \sqrt{A_{22} - L_{21}^2}$
- $A_{31} \rightarrow A_{31}/L_{11}$
- $A_{32} \rightarrow (A_{32} - L_{31}L_{21})/L_{22}$
- $A_{33} \rightarrow \sqrt{A_{33} - L_{31}^2 - L_{32}^2}$

$$\text{Order of computation} = \begin{pmatrix} 1 \\ 2 & 3 \\ 2 & 4 & 5 \\ 2 & 6 & 7 & 8 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 1 \\ 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 & 10 \end{pmatrix}$$

General formula to compute  $L$ :

$$L_{i,j} = \begin{cases} \sqrt{A_{1,1}} & j=1, i=1 \\ A_{i,1} / L_{1,1} & j=1, i>1 \\ 0 & i < j \\ \sqrt{A_{i,j} - \sum_{k=1, \dots, j-1} L_{j,k}^2} & i=j \\ \frac{1}{L_{j,j}} \cdot \left( A_{i,j} - \sum_{k=1, \dots, j-1} L_{i,k} \cdot L_{j,k} \right) & i > j \end{cases}$$

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# Overview

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1. Questions and Updates
2. Recap: Unit 7, Linear Algebra, and the Inverse of a Matrix
3. Recap: Cholesky Decomposition
- 4. Recap: Linear Regression in Matrix Notation**

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## Recap: Regression & Linear Basis Function Models

Dependent variable  $y$

Explanatory variables  $x_0, x_1, \dots, x_K$

Model: Find weights such that  $\beta_0 \cdot x_0 + \beta_1 \cdot x_1 + \dots + \beta_K \cdot x_K = \sum_{k=0,1,\dots,K} \beta_k \cdot x_k \approx y$

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## Recap: Regression & Linear Basis Function Models

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Data (Example):  $y_i, z_i = (a_i, b_i) \quad i = 1, \dots, n$

Basis Functions: (i)  $y_i \approx \beta_0 + \beta_1 \cdot a_i + \beta_2 \cdot b_i + \beta_3 \cdot \sqrt{a_i \cdot b_i}$

(ii)

(iii)

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# Recap: Regression & Linear Basis Function Models

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(ii)  $y_i \approx \beta_0 + \beta_1 \cdot a_i + \beta_2 \cdot a_i^2 + \dots + \beta_K \cdot a_i^K$

(iii)

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# Recap: Regression & Linear Basis Function Models

Dependent variable  $y$

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Data (Example):  $y_i, z_i = (a_i, b_i) \quad i = 1, \dots, n$

Basis Functions: (i)  $y_i \approx \beta_0 + \beta_1 \cdot a_i + \beta_2 \cdot b_i + \beta_3 \cdot \sqrt{a_i \cdot b_i}$

(ii)  $y_i \approx \beta_0 + \beta_1 \cdot a_i + \beta_2 \cdot a_i^2 + \dots + \beta_K \cdot a_i^K$

(iii)  $y_i \approx \beta_0 + \beta_1 \cdot a_i + \beta_2 \cdot a_i^2 + \dots + \beta_K \cdot a_i^K$   
 $+ \beta_{K+1} \cdot b_i + \beta_{K+2} \cdot b_i^2 + \dots + \beta_{K+K} \cdot b_i^K$

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# Recap: Regression & Linear Basis Function Models

Dependent variable  $y$

Explanatory variables  $x_0, x_1, \dots, x_K$

Model: Find weights such that  $\beta_0 \cdot x_0 + \beta_1 \cdot x_1 + \dots + \beta_K \cdot x_K = \sum_{k=0,1,\dots,K} \beta_k \cdot x_k \approx y$

Data (Example):  $y_i, z_i = (a_i, b_i) \quad i = 1, \dots, n$

Basis Functions: (i)  $y_i \approx \beta_0 + \beta_1 \cdot a_i + \beta_2 \cdot b_i + \beta_3 \cdot \sqrt{a_i \cdot b_i} \longrightarrow \sum_{k=0,1,\dots,3} \beta_k \cdot x_k^{(i)} \approx y_i$

(ii)  $y_i \approx \beta_0 + \beta_1 \cdot a_i + \beta_2 \cdot a_i^2 + \dots + \beta_K \cdot a_i^K \longrightarrow \sum_{k=0,1,\dots,K} \beta_k \cdot x_k^{(i)} \approx y_i$

(iii)  $y_i \approx \beta_0 + \beta_1 \cdot a_i + \beta_2 \cdot a_i^2 + \dots + \beta_K \cdot a_i^K + \beta_{K+1} \cdot b_i + \beta_{K+2} \cdot b_i^2 + \dots + \beta_{K+K} \cdot b_i^K \longrightarrow \sum_{k=0,1,\dots,2K} \beta_k \cdot x_k^{(i)} \approx y_i$

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## Recap: Linear Regression

Dependent variable  $y$

Explanatory variables  $x_0, x_1, \dots, x_K$  (cf. Basis function models)

Model: Find weights such that  $\beta_0 \cdot x_0 + \beta_1 \cdot x_1 + \dots + \beta_K \cdot x_K = \sum_{k=0,1,\dots,K} \beta_k \cdot x_k \approx y$

**Objective of the Regression?** What are the variables?

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## Recap: Linear Regression

Dependent variable  $y$

Explanatory variables  $x_0, x_1, \dots, x_K$  (cf. Basis function models)

Model: Find weights such that  $\beta_0 \cdot x_0 + \beta_1 \cdot x_1 + \dots + \beta_K \cdot x_K = \sum_{k=0,1,\dots,K} \beta_k \cdot x_k \approx y$

**Minimize the Sum of Squared Errors:**

$$\begin{aligned} & \min_{\beta_k \in \mathbb{R}, k=0,\dots,K} \sum_{i=1,\dots,N} \left( \beta_0 \cdot x_{0,i} + \beta_1 \cdot x_{1,i} + \dots + \beta_K \cdot x_{K,i} - y_i \right)^2 \\ & \simeq \vec{\beta}^* := \arg \min_{\vec{\beta} \in \mathbb{R}^{K+1}} \sum_{i=1,\dots,N} \underbrace{\left( y_i - \sum_{j=1,\dots,K} \beta_j \cdot x_{j,i} \right)^2}_{\text{errors } \varepsilon_i} \end{aligned}$$

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## Let's take a Look: Residuals and Matrix Notation

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n$

What is happening here in Matrix Notation?

# Let's take a Look: Residuals and Matrix Notation

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n$

What is happening here in Matrix Notation?

We have:

$$\begin{pmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{pmatrix}_{n \times 1} = \begin{pmatrix} 1 & x_{1,1} & x_{2,1} & \dots & x_{K,1} \\ 1 & x_{1,2} & x_{2,2} & & x_{K,2} \\ \dots & & & & \\ 1 & x_{1,n} & x_{2,n} & & x_{K,n} \end{pmatrix}_{n \times (K+1)} \cdot \begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_K \end{pmatrix}_{(K+1) \times 1} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \dots \\ \varepsilon_n \end{pmatrix}_{n \times 1}$$

Or just ??

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# Let's take a Look: Residuals and Matrix Notation

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n$

What is happening here in Matrix Notation?

We have:

$$\begin{pmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{pmatrix}_{n \times 1} = \begin{pmatrix} 1 & x_{1,1} & x_{2,1} & \dots & x_{K,1} \\ 1 & x_{1,2} & x_{2,2} & & x_{K,2} \\ \dots & & & & \\ 1 & x_{1,n} & x_{2,n} & & x_{K,n} \end{pmatrix}_{n \times (K+1)} \cdot \begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_K \end{pmatrix}_{(K+1) \times 1} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \dots \\ \varepsilon_n \end{pmatrix}_{n \times 1}$$

Or just:  $\vec{y} = X\vec{\beta} + \vec{\varepsilon} \quad \Leftrightarrow \quad \vec{\varepsilon} = \vec{y} - X\vec{\beta}$

# Sum of Squared Errors

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n \quad \text{or} \quad \vec{\varepsilon} = \vec{y} - X\vec{\beta}$

Sum of squared errors in Matrix notation?

# Sum of Squared Errors

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n \quad \text{or} \quad \vec{\varepsilon} = \vec{y} - X\vec{\beta}$

Sum of squared errors:

$$\begin{pmatrix} \varepsilon_1 & \varepsilon_2 & \dots & \varepsilon_n \end{pmatrix}_{1 \times n} \cdot \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \dots \\ \varepsilon_n \end{pmatrix}_{n \times 1} = \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 = \vec{\varepsilon}^T \vec{\varepsilon}$$

Great! What now?

# Sum of Squared Errors

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n \quad \text{or} \quad \vec{\varepsilon} = \vec{y} - X\vec{\beta}$

Sum of squared errors:

$$\begin{pmatrix} \varepsilon_1 & \varepsilon_2 & \dots & \varepsilon_n \end{pmatrix}_{1 \times n} \cdot \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \dots \\ \varepsilon_n \end{pmatrix}_{n \times 1} = \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 = \vec{\varepsilon}^T \vec{\varepsilon}$$

We have:

$$\begin{aligned} \vec{\varepsilon}^T \vec{\varepsilon} &= (\vec{y} - X\vec{\beta})^T \cdot (\vec{y} - X\vec{\beta}) \\ &= ?? \end{aligned}$$

# Sum of Squared Errors

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n \quad \text{or} \quad \vec{\varepsilon} = \vec{y} - X\vec{\beta}$

Sum of squared errors:

$$\begin{pmatrix} \varepsilon_1 & \varepsilon_2 & \dots & \varepsilon_n \end{pmatrix}_{1 \times n} \cdot \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \dots \\ \varepsilon_n \end{pmatrix}_{n \times 1} = \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 = \vec{\varepsilon}^T \vec{\varepsilon}$$

We have:

$$\begin{aligned} \vec{\varepsilon}^T \vec{\varepsilon} &= (\vec{y} - X\vec{\beta})^T \cdot (\vec{y} - X\vec{\beta}) \\ &= (\vec{y}^T - (X\vec{\beta})^T) \cdot (\vec{y} - X\vec{\beta}) \\ &= ?? \end{aligned}$$


# Sum of Squared Errors

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n \quad \text{or} \quad \vec{\varepsilon} = \vec{y} - X\vec{\beta}$

Sum of squared errors:

$$(\varepsilon_1 \quad \varepsilon_2 \quad \dots \quad \varepsilon_n)_{1 \times n} \cdot \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \dots \\ \varepsilon_n \end{pmatrix}_{n \times 1} = \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 = \vec{\varepsilon}^T \vec{\varepsilon}$$

We have:

$$\begin{aligned} \vec{\varepsilon}^T \vec{\varepsilon} &= (\vec{y} - X\vec{\beta})^T \cdot (\vec{y} - X\vec{\beta}) \\ &= (\vec{y}^T - (X\vec{\beta})^T) \cdot (\vec{y} - X\vec{\beta}) \\ &= \vec{y}^T \vec{y} - \vec{y}^T X\vec{\beta} - (X\vec{\beta})^T \vec{y} + (X\vec{\beta})^T X\vec{\beta} \end{aligned}$$


# Transposed Terms

Consider:

$$X\vec{\beta} = \begin{pmatrix} 1 & x_{1,1} & x_{2,1} & \dots & x_{K,1} \\ 1 & x_{1,2} & x_{2,2} & & x_{K,2} \\ \dots & & & \dots & \\ 1 & x_{1,n} & x_{2,n} & & x_{K,n} \end{pmatrix}_{n \times (K+1)} \cdot \begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_K \end{pmatrix}_{(K+1) \times 1} = \begin{pmatrix} \vec{x}_1^T \vec{\beta} \\ \vec{x}_2^T \vec{\beta} \\ \dots \\ \vec{x}_n^T \vec{\beta} \end{pmatrix}_{n \times 1}$$

Then:  $(X\vec{\beta})^T = ??$

## Transposed Terms

Consider:

$$X\vec{\beta} = \begin{pmatrix} 1 & x_{1,1} & x_{2,1} & \dots & x_{K,1} \\ 1 & x_{1,2} & x_{2,2} & & x_{K,2} \\ \dots & & & \dots & \\ 1 & x_{1,n} & x_{2,n} & & x_{K,n} \end{pmatrix}_{n \times (K+1)} \cdot \begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_K \end{pmatrix}_{(K+1) \times 1} = \begin{pmatrix} \vec{x}_1^T \vec{\beta} \\ \vec{x}_2^T \vec{\beta} \\ \dots \\ \vec{x}_n^T \vec{\beta} \end{pmatrix}_{n \times 1}$$

Then:

$$(X\vec{\beta})^T = \begin{pmatrix} \vec{x}_1^T \vec{\beta} & \vec{x}_2^T \vec{\beta} & \dots & \vec{x}_n^T \vec{\beta} \end{pmatrix}_{1 \times n} = ??$$



# Transposed Terms

Consider:

$$X\vec{\beta} = \begin{pmatrix} 1 & x_{1,1} & x_{2,1} & \dots & x_{K,1} \\ 1 & x_{1,2} & x_{2,2} & & x_{K,2} \\ \dots & & & \dots & \\ 1 & x_{1,n} & x_{2,n} & & x_{K,n} \end{pmatrix}_{n \times (K+1)} \cdot \begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_K \end{pmatrix}_{(K+1) \times 1} = \begin{pmatrix} \vec{x}_1^T \vec{\beta} \\ \vec{x}_2^T \vec{\beta} \\ \dots \\ \vec{x}_n^T \vec{\beta} \end{pmatrix}_{n \times 1}$$

We have:

$$(X\vec{\beta})^T = \begin{pmatrix} \vec{x}_1^T \vec{\beta} & \vec{x}_2^T \vec{\beta} & \dots & \vec{x}_n^T \vec{\beta} \end{pmatrix}_{1 \times n} = \begin{pmatrix} \beta_0 & \beta_1 & \dots & \beta_K \end{pmatrix}_{1 \times (K+1)} \cdot \begin{pmatrix} 1 & 1 & \dots & 1 \\ x_{1,1} & x_{1,2} & & x_{1,n} \\ x_{2,1} & x_{2,2} & & x_{2,n} \\ \dots & & \dots & \\ x_{K,1} & x_{K,2} & & x_{K,n} \end{pmatrix}_{(K+1) \times n}$$

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## Transposed Terms

Consider:

$$X\vec{\beta} = \begin{pmatrix} 1 & x_{1,1} & x_{2,1} & \dots & x_{K,1} \\ 1 & x_{1,2} & x_{2,2} & & x_{K,2} \\ \dots & & & \dots & \\ 1 & x_{1,n} & x_{2,n} & & x_{K,n} \end{pmatrix}_{n \times (K+1)} \cdot \begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_K \end{pmatrix}_{(K+1) \times 1} = \begin{pmatrix} \vec{x}_1^T \vec{\beta} \\ \vec{x}_2^T \vec{\beta} \\ \dots \\ \vec{x}_n^T \vec{\beta} \end{pmatrix}_{n \times 1}$$

We have:

$$(X\vec{\beta})^T = \begin{pmatrix} \vec{x}_1^T \vec{\beta} & \vec{x}_2^T \vec{\beta} & \dots & \vec{x}_n^T \vec{\beta} \end{pmatrix}_{1 \times n} = \begin{pmatrix} \beta_0 & \beta_1 & \dots & \beta_K \end{pmatrix}_{1 \times (K+1)} \cdot \begin{pmatrix} 1 & 1 & \dots & 1 \\ x_{1,1} & x_{1,2} & & x_{1,n} \\ x_{2,1} & x_{2,2} & & x_{2,n} \\ \dots & & \dots & \\ x_{K,1} & x_{K,2} & & x_{K,n} \end{pmatrix}_{(K+1) \times n}$$

$$= \vec{\beta}^T X^T$$

Note: Switch the order!

# Sum of Squared Errors

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n \quad \text{or} \quad \vec{\varepsilon} = \vec{y} - X\vec{\beta}$

Sum of squared errors:  $\varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 = \vec{\varepsilon}^T \vec{\varepsilon}$

We have:

$$\begin{aligned}
 \vec{\varepsilon}^T \vec{\varepsilon} &= (\vec{y} - X\vec{\beta})^T \cdot (\vec{y} - X\vec{\beta}) \\
 &= (\vec{y}^T - (X\vec{\beta})^T) \cdot (\vec{y} - X\vec{\beta}) \\
 &= \vec{y}^T \vec{y} - \vec{y}^T X\vec{\beta} - \boxed{(X\vec{\beta})^T \vec{y}} + (X\vec{\beta})^T X\vec{\beta} \\
 &= \vec{y}^T \vec{y} - \vec{y}^T X\vec{\beta} - \vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X\vec{\beta} \\
 &= ??
 \end{aligned}$$

# Sum of Squared Errors

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n \quad \text{or} \quad \vec{\varepsilon} = \vec{y} - X\vec{\beta}$

Sum of squared errors:  $\varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 = \vec{\varepsilon}^T \vec{\varepsilon}$

We have:

$$\begin{aligned}
 \vec{\varepsilon}^T \vec{\varepsilon} &= (\vec{y} - X\vec{\beta})^T \cdot (\vec{y} - X\vec{\beta}) \\
 &= (\vec{y}^T - (X\vec{\beta})^T) \cdot (\vec{y} - X\vec{\beta}) \\
 &= \vec{y}^T \vec{y} - \vec{y}^T X\vec{\beta} - (X\vec{\beta})^T \vec{y} + (X\vec{\beta})^T X\vec{\beta} \\
 &= \vec{y}^T \vec{y} - \vec{y}^T X\vec{\beta} - \vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X\vec{\beta} \\
 &= \vec{y}^T \vec{y} - \underbrace{(\vec{y}^T X\vec{\beta})^T}_{\in \mathbb{R}} - \vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X\vec{\beta} \\
 &= ??
 \end{aligned}$$

# Sum of Squared Errors

Consider the errors:  $\varepsilon_i := y_i - \sum_{k=0,1,\dots,K} \beta_k \cdot x_{k,i} \quad i=1,\dots,n \quad \text{or} \quad \vec{\varepsilon} = \vec{y} - X\vec{\beta}$

Sum of squared errors:  $\varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 = \vec{\varepsilon}^T \vec{\varepsilon}$

We have:

$$\begin{aligned}
 \vec{\varepsilon}^T \vec{\varepsilon} &= (\vec{y} - X\vec{\beta})^T \cdot (\vec{y} - X\vec{\beta}) \\
 &= (\vec{y}^T - (X\vec{\beta})^T) \cdot (\vec{y} - X\vec{\beta}) \\
 &= \vec{y}^T \vec{y} - \vec{y}^T X\vec{\beta} - (X\vec{\beta})^T \vec{y} + (X\vec{\beta})^T X\vec{\beta} \\
 &= \vec{y}^T \vec{y} - \vec{y}^T X\vec{\beta} - \vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X\vec{\beta} \\
 &= \vec{y}^T \vec{y} - \boxed{(\vec{y}^T X\vec{\beta})^T} - \vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X\vec{\beta} \\
 &= \vec{y}^T \vec{y} - \boxed{\vec{\beta}^T X^T \vec{y}} - \vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X\vec{\beta} \\
 &= \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X\vec{\beta}
 \end{aligned}$$

# Minimizing the Sum of Squared Errors

Sum of squared errors:  $\vec{\varepsilon}^T \vec{\varepsilon} = \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta} \in \mathbb{R}$

Derivatives/FOC??

# Minimizing the Sum of Squared Errors

Sum of squared errors:  $\vec{\varepsilon}^T \vec{\varepsilon} = \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta} \in \mathbb{R}$

Derivatives/FOC:  $\frac{\partial}{\partial \beta_k} \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 \quad \forall k = 0, 1, \dots, K \Rightarrow$

Hence:  $\frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} = ??$

$$\begin{pmatrix} \frac{\partial}{\partial \beta_0} \vec{\varepsilon}^T \vec{\varepsilon} \\ \frac{\partial}{\partial \beta_1} \vec{\varepsilon}^T \vec{\varepsilon} \\ \dots \\ \frac{\partial}{\partial \beta_K} \vec{\varepsilon}^T \vec{\varepsilon} \end{pmatrix}_{(K+1) \times 1} = \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} \stackrel{!}{=} \vec{0}$$

# Minimizing the Sum of Squared Errors

Sum of squared errors:  $\vec{\varepsilon}^T \vec{\varepsilon} = \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta} \in \mathbb{R}$

Derivatives/FOC:  $\frac{\partial}{\partial \beta_k} \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 \quad \forall k = 0, 1, \dots, K \Rightarrow$

$$\begin{pmatrix} \frac{\partial}{\partial \beta_0} \vec{\varepsilon}^T \vec{\varepsilon} \\ \frac{\partial}{\partial \beta_1} \vec{\varepsilon}^T \vec{\varepsilon} \\ \dots \\ \frac{\partial}{\partial \beta_K} \vec{\varepsilon}^T \vec{\varepsilon} \end{pmatrix}_{(K+1) \times 1} = \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} \stackrel{!}{=} \vec{0}$$

Hence: 
$$\begin{aligned} \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} &= \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta}) \\ &= \underbrace{\frac{\partial}{\partial \vec{\beta}} \vec{y}^T \vec{y}}_{??} - \frac{\partial}{\partial \vec{\beta}} 2\vec{\beta}^T X^T \vec{y} + \frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta} \end{aligned}$$






# Minimizing the Sum of Squared Errors

Sum of squared errors:  $\vec{\varepsilon}^T \vec{\varepsilon} = \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta} \in \mathbb{R}$

Derivatives/FOC:  $\frac{\partial}{\partial \beta_k} \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 \quad \forall k = 0, 1, \dots, K \Rightarrow \begin{pmatrix} \frac{\partial}{\partial \beta_0} \vec{\varepsilon}^T \vec{\varepsilon} \\ \frac{\partial}{\partial \beta_1} \vec{\varepsilon}^T \vec{\varepsilon} \\ \dots \\ \frac{\partial}{\partial \beta_K} \vec{\varepsilon}^T \vec{\varepsilon} \end{pmatrix}_{(K+1) \times 1} = \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} \stackrel{!}{=} \vec{0}$

Hence: 
$$\begin{aligned} \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} &= \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta}) \\ &= \underbrace{\frac{\partial}{\partial \vec{\beta}} \vec{y}^T \vec{y}}_{\begin{pmatrix} 0 \\ 0 \\ \dots \\ 0 \end{pmatrix}_{(K+1) \times 1}} - \frac{\partial}{\partial \vec{\beta}} 2\vec{\beta}^T X^T \vec{y} + \frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta} \end{aligned}$$

  $\boxed{\frac{\partial}{\partial \beta_k}} \vec{y}^T \vec{y} = \frac{\partial}{\partial \beta_k} (y_1^2 + y_2^2 + \dots + y_n^2) = 0 \quad \forall k = 0, 1, \dots, K$

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# Minimizing the Sum of Squared Errors

Sum of squared errors:  $\vec{\varepsilon}^T \vec{\varepsilon} = \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta} \in \mathbb{R}$

Derivatives/FOC:  $\frac{\partial}{\partial \beta_k} \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 \quad \forall k = 0, 1, \dots, K \Rightarrow$

$$\begin{pmatrix} \frac{\partial}{\partial \beta_0} \vec{\varepsilon}^T \vec{\varepsilon} \\ \frac{\partial}{\partial \beta_1} \vec{\varepsilon}^T \vec{\varepsilon} \\ \dots \\ \frac{\partial}{\partial \beta_K} \vec{\varepsilon}^T \vec{\varepsilon} \end{pmatrix}_{(K+1) \times 1} = \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} \stackrel{!}{=} \vec{0}$$

Hence: 
$$\frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} = \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta})$$

$$= \vec{0} - \underbrace{\frac{\partial}{\partial \vec{\beta}} 2\vec{\beta}^T X^T \vec{y}}_{??} + \frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta}$$


# Minimizing the Sum of Squared Errors

Sum of squared errors:  $\vec{\varepsilon}^T \vec{\varepsilon} = \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta} \in \mathbb{R}$

Derivatives/FOC:  $\frac{\partial}{\partial \beta_k} \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 \quad \forall k = 0, 1, \dots, K \Rightarrow$

$$\begin{pmatrix} \frac{\partial}{\partial \beta_0} \vec{\varepsilon}^T \vec{\varepsilon} \\ \frac{\partial}{\partial \beta_1} \vec{\varepsilon}^T \vec{\varepsilon} \\ \dots \\ \frac{\partial}{\partial \beta_K} \vec{\varepsilon}^T \vec{\varepsilon} \end{pmatrix}_{(K+1) \times 1} = \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} \stackrel{!}{=} \vec{0}$$

Hence:  $\frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} = \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta})$

$$= \vec{0} - \underbrace{\frac{\partial}{\partial \vec{\beta}} 2\vec{\beta}^T X^T \vec{y}}_{2X^T \vec{y}} + \frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta}$$

$$\boxed{\frac{\partial}{\partial \beta_k}} 2\vec{\beta}_{1 \times (K+1)}^T \underbrace{X^T \vec{y}}_{\vec{m} \quad (K+1) \times 1} = ??$$

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# Minimizing the Sum of Squared Errors

Sum of squared errors:  $\vec{\varepsilon}^T \vec{\varepsilon} = \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta} \in \mathbb{R}$

Derivatives/FOC:  $\frac{\partial}{\partial \beta_k} \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 \quad \forall k = 0, 1, \dots, K \Rightarrow$

$$\begin{pmatrix} \frac{\partial}{\partial \beta_0} \vec{\varepsilon}^T \vec{\varepsilon} \\ \frac{\partial}{\partial \beta_1} \vec{\varepsilon}^T \vec{\varepsilon} \\ \dots \\ \frac{\partial}{\partial \beta_K} \vec{\varepsilon}^T \vec{\varepsilon} \end{pmatrix}_{(K+1) \times 1} = \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} \stackrel{!}{=} \vec{0}$$

Hence:  $\frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} = \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta})$

$$= \vec{0} - \underbrace{\frac{\partial}{\partial \vec{\beta}} 2\vec{\beta}^T X^T \vec{y}}_{2X^T \vec{y}} + \frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta}$$

$$\frac{\partial}{\partial \beta_k} 2\vec{\beta}_{1 \times (K+1)}^T \underbrace{X^T \vec{y}}_{\vec{m} \quad (K+1) \times 1} = 2 \frac{\partial}{\partial \beta_k} (\beta_0 \cdot m_0 + \beta_1 \cdot m_1 + \dots + \beta_K \cdot m_K) = ??$$

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# Minimizing the Sum of Squared Errors

Sum of squared errors:  $\vec{\varepsilon}^T \vec{\varepsilon} = \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta} \in \mathbb{R}$

Derivatives/FOC:  $\frac{\partial}{\partial \beta_k} \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 \quad \forall k = 0, 1, \dots, K \Rightarrow$

$$\begin{pmatrix} \frac{\partial}{\partial \beta_0} \vec{\varepsilon}^T \vec{\varepsilon} \\ \frac{\partial}{\partial \beta_1} \vec{\varepsilon}^T \vec{\varepsilon} \\ \dots \\ \frac{\partial}{\partial \beta_K} \vec{\varepsilon}^T \vec{\varepsilon} \end{pmatrix}_{(K+1) \times 1} = \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} \stackrel{!}{=} \vec{0}$$


Hence:  $\frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} = \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta})$

$$= \vec{0} - \underbrace{\frac{\partial}{\partial \vec{\beta}} 2\vec{\beta}^T X^T \vec{y}}_{2X^T \vec{y}} + \frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta}$$

$$\frac{\partial}{\partial \beta_k} 2\vec{\beta}_{1 \times (K+1)}^T \underbrace{X^T \vec{y}}_{\vec{m} \quad (K+1) \times 1} = 2 \frac{\partial}{\partial \beta_k} (\beta_0 \cdot m_0 + \beta_1 \cdot m_1 + \dots + \beta_K \cdot m_K) = 2 \cdot m_k \quad \forall k = 0, 1, \dots, K$$

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# Minimizing the Sum of Squared Errors


Hence: 
$$\frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} = \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta})$$
$$= \vec{0} - 2X^T \vec{y} + \underbrace{\frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta}}_{(K+1) \times 1}$$


# Minimizing the Sum of Squared Errors

$$\boxed{\frac{\partial}{\partial \beta_k}} \underbrace{\vec{\beta}^T}_{1 \times (K+1)} \underbrace{X^T X}_{(K+1) \times (K+1)} \underbrace{\vec{\beta}}_{(K+1) \times 1} = \frac{\partial}{\partial \beta_k} \underbrace{\vec{\beta}^T}_{1 \times (K+1)} \cdot \begin{pmatrix} \beta_0 \cdot m_{0,0} & +\beta_1 \cdot m_{0,1} & \dots & +\beta_K \cdot m_{0,K} \\ \beta_0 \cdot m_{1,0} & +\beta_1 \cdot m_{1,1} & \dots & +\beta_K \cdot m_{1,K} \\ & & \dots & \\ \beta_0 \cdot m_{K,0} & +\beta_1 \cdot m_{K,1} & \dots & +\beta_K \cdot m_{K,K} \end{pmatrix} = ??$$

$\begin{pmatrix} \vec{m}_0^T \\ \vec{m}_1^T \\ \dots \\ \vec{m}_K^T \end{pmatrix}$

Hence: 
$$\frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} = \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta})$$


$$= \vec{0} - 2X^T \vec{y} + \underbrace{\frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta}}_{(K+1) \times 1}$$


# Minimizing the Sum of Squared Errors

$$\frac{\partial}{\partial \beta_k} \underbrace{\vec{\beta}^T}_{1 \times (K+1)} \underbrace{X^T X}_{(K+1) \times (K+1)} \underbrace{\vec{\beta}}_{(K+1) \times 1} = \frac{\partial}{\partial \beta_k} \underbrace{\vec{\beta}^T}_{1 \times (K+1)} \cdot \begin{pmatrix} \beta_0 \cdot m_{0,0} & +\beta_1 \cdot m_{0,1} & \dots & +\beta_K \cdot m_{0,K} \\ \beta_0 \cdot m_{1,0} & +\beta_1 \cdot m_{1,1} & \dots & +\beta_K \cdot m_{1,K} \\ & & \dots & \\ \beta_0 \cdot m_{K,0} & +\beta_1 \cdot m_{K,1} & \dots & +\beta_K \cdot m_{K,K} \end{pmatrix} = \frac{\partial}{\partial \beta_k} \begin{pmatrix} \beta_0 \cdot (\beta_0 \cdot m_{0,0} + \beta_1 \cdot m_{0,1} + \dots + \beta_K \cdot m_{0,K}) \\ +\beta_1 \cdot (\beta_0 \cdot m_{1,0} + \beta_1 \cdot m_{1,1} + \dots + \beta_K \cdot m_{1,K}) \\ \dots \\ +\beta_K \cdot (\beta_0 \cdot m_{K,0} + \beta_1 \cdot m_{K,1} + \dots + \beta_K \cdot m_{K,K}) \end{pmatrix}$$


$\begin{pmatrix} \vec{m}_0^T \\ \vec{m}_1^T \\ \dots \\ \vec{m}_K^T \end{pmatrix}$

Hence: 
$$\frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} = \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2 \vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta})$$

$$= \vec{0} - 2X^T \vec{y} + \underbrace{\frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta}}_{(K+1) \times 1}$$




# Minimizing the Sum of Squared Errors

$$\begin{aligned}
 \frac{\partial}{\partial \beta_k} \underbrace{\vec{\beta}^T}_{1 \times (K+1)} \underbrace{X^T X}_{(K+1) \times (K+1)} \underbrace{\vec{\beta}}_{(K+1) \times 1} &= \frac{\partial}{\partial \beta_k} \vec{\beta}^T \cdot \begin{pmatrix} \beta_0 \cdot m_{0,0} & +\beta_1 \cdot m_{0,1} & \dots & +\beta_K \cdot m_{0,K} \\ \beta_0 \cdot m_{1,0} & +\beta_1 \cdot m_{1,1} & \dots & +\beta_K \cdot m_{1,K} \\ & & \dots & \\ \beta_0 \cdot m_{K,0} & +\beta_1 \cdot m_{K,1} & \dots & +\beta_K \cdot m_{K,K} \end{pmatrix} = \frac{\partial}{\partial \beta_k} \begin{pmatrix} \beta_0 \cdot (\beta_0 \cdot m_{0,0} + \beta_1 \cdot m_{0,1} + \dots + \beta_K \cdot m_{0,K}) \\ +\beta_1 \cdot (\beta_0 \cdot m_{1,0} + \beta_1 \cdot m_{1,1} + \dots + \beta_K \cdot m_{1,K}) \\ \dots \\ +\beta_K \cdot (\beta_0 \cdot m_{K,0} + \beta_1 \cdot m_{K,1} + \dots + \beta_K \cdot m_{K,K}) \end{pmatrix} \\
 \text{Hence: } \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} &= \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta}) \\
 &= \vec{0} - 2X^T \vec{y} + \underbrace{\frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta}}_{(K+1) \times 1}
 \end{aligned}$$


# Minimizing the Sum of Squared Errors

$$\begin{aligned}
 \frac{\partial}{\partial \beta_k} \underbrace{\vec{\beta}^T}_{1 \times (K+1)} \underbrace{X^T X}_{(K+1) \times (K+1)} \underbrace{\vec{\beta}}_{(K+1) \times 1} &= \frac{\partial}{\partial \beta_k} \vec{\beta}^T \cdot \begin{pmatrix} \beta_0 \cdot m_{0,0} & +\beta_1 \cdot m_{0,1} & \dots & +\beta_K \cdot m_{0,K} \\ \beta_0 \cdot m_{1,0} & +\beta_1 \cdot m_{1,1} & \dots & +\beta_K \cdot m_{1,K} \\ & & \dots & \\ \beta_0 \cdot m_{K,0} & +\beta_1 \cdot m_{K,1} & \dots & +\beta_K \cdot m_{K,K} \end{pmatrix} = \frac{\partial}{\partial \beta_k} \begin{pmatrix} \beta_0 \cdot (\beta_0 \cdot m_{0,0} + \beta_1 \cdot m_{0,1} + \dots + \beta_K \cdot m_{0,K}) \\ +\beta_1 \cdot (\beta_0 \cdot m_{1,0} + \beta_1 \cdot m_{1,1} + \dots + \beta_K \cdot m_{1,K}) \\ \dots \\ +\beta_K \cdot (\beta_0 \cdot m_{K,0} + \beta_1 \cdot m_{K,1} + \dots + \beta_K \cdot m_{K,K}) \end{pmatrix} \\
 \text{Hence: } \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} &= \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta}) \\
 &= \vec{0} - 2X^T \vec{y} + \frac{\partial}{\partial \vec{\beta}} \underbrace{\vec{\beta}^T X^T X \vec{\beta}}_{\substack{2X^T X \vec{\beta} \\ (K+1) \times 1}} \\
 &= \underbrace{X^T X \text{ symmetric}}_{m_{k,i} = m_{i,k}, \forall i, k=0,1,\dots,K} \cdot 2 \cdot (\beta_0 \cdot m_{k,0} + \beta_1 \cdot m_{k,1} + \dots + \beta_K \cdot m_{k,K}) \\
 &= 2 \cdot k^{\text{th}} \text{ row of } X^T X \vec{\beta} \quad \forall k = 0, 1, \dots, K
 \end{aligned}$$

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# Minimizing the Sum of Squared Errors

Sum of squared errors:  $\vec{\varepsilon}^T \vec{\varepsilon} = \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta} \in \mathbb{R}$

Derivatives/FOC:  $\frac{\partial}{\partial \beta_k} \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 \quad \forall k = 0, 1, \dots, K \Rightarrow$

$$\begin{pmatrix} \frac{\partial}{\partial \beta_0} \vec{\varepsilon}^T \vec{\varepsilon} \\ \frac{\partial}{\partial \beta_1} \vec{\varepsilon}^T \vec{\varepsilon} \\ \dots \\ \frac{\partial}{\partial \beta_K} \vec{\varepsilon}^T \vec{\varepsilon} \end{pmatrix}_{(K+1) \times 1} = \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} \stackrel{!}{=} \vec{0}$$

Hence: 
$$\begin{aligned} \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} &= \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta}) \\ &= \frac{\partial}{\partial \vec{\beta}} \vec{y}^T \vec{y} - \frac{\partial}{\partial \vec{\beta}} 2\vec{\beta}^T X^T \vec{y} + \frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta} \\ &= -2X^T \vec{y} + 2X^T X \vec{\beta} \stackrel{!}{=} \vec{0} \end{aligned}$$

# Minimizing the Sum of Squared Errors

Sum of squared errors:  $\vec{\varepsilon}^T \vec{\varepsilon} = \vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta} \in \mathbb{R}$

Derivatives/FOC:  $\frac{\partial}{\partial \beta_k} \varepsilon_1^2 + \varepsilon_2^2 + \dots + \varepsilon_n^2 \quad \forall k = 0, 1, \dots, K \Rightarrow$

$$\begin{pmatrix} \frac{\partial}{\partial \beta_0} \vec{\varepsilon}^T \vec{\varepsilon} \\ \frac{\partial}{\partial \beta_1} \vec{\varepsilon}^T \vec{\varepsilon} \\ \dots \\ \frac{\partial}{\partial \beta_K} \vec{\varepsilon}^T \vec{\varepsilon} \end{pmatrix}_{(K+1) \times 1} = \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} \stackrel{!}{=} \vec{0}$$

Hence:

$$\begin{aligned} \frac{\partial \vec{\varepsilon}^T \vec{\varepsilon}}{\partial \vec{\beta}} &= \frac{\partial}{\partial \vec{\beta}} (\vec{y}^T \vec{y} - 2\vec{\beta}^T X^T \vec{y} + \vec{\beta}^T X^T X \vec{\beta}) \\ &= \frac{\partial}{\partial \vec{\beta}} \vec{y}^T \vec{y} - \frac{\partial}{\partial \vec{\beta}} 2\vec{\beta}^T X^T \vec{y} + \frac{\partial}{\partial \vec{\beta}} \vec{\beta}^T X^T X \vec{\beta} \\ &= -2X^T \vec{y} + 2X^T X \vec{\beta} \stackrel{!}{=} \vec{0} \end{aligned}$$

$$\Leftrightarrow X^T X \vec{\beta} \stackrel{!}{=} X^T \vec{y}$$

What do we want again?

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# Minimizing the Sum of Squared Errors

Optimality condition:

$$\underbrace{X^T}_{(K+1) \times \dots} X \underbrace{\vec{\beta}}_{\dots \times 1} \stackrel{!}{=} \underbrace{X^T \vec{y}}_{(K+1) \times 1}$$

How to get the optimal weights  $\vec{\beta}$  ?

Any ideas?

# Minimizing the Sum of Squared Errors

Optimality condition:

$$\underbrace{X^T}_{(K+1) \times \dots} X \underbrace{\vec{\beta}}_{\dots \times 1} \stackrel{!}{=} \underbrace{X^T \vec{y}}_{(K+1) \times 1}$$

How to get the optimal weights  $\vec{\beta}$  ?

If  $X^T X$  has full rank, then the inverse exists and we get:

$$\Leftrightarrow (X^T X)^{-1} \cdot X^T X \vec{\beta} = (X^T X)^{-1} \cdot X^T \vec{y}$$

# Minimizing the Sum of Squared Errors

Optimality condition:

$$\underbrace{X^T}_{(K+1) \times \dots} X \underbrace{\vec{\beta}}_{\dots \times 1} \stackrel{!}{=} \underbrace{X^T \vec{y}}_{(K+1) \times 1}$$

How to get the optimal weights  $\vec{\beta}$  ?

If  $X^T X$  has full rank, then the inverse exists and we get:

$$\Leftrightarrow (X^T X)^{-1} \cdot X^T X \vec{\beta} = (X^T X)^{-1} \cdot X^T \vec{y}$$

$$\Leftrightarrow I \cdot \vec{\beta} = (X^T X)^{-1} \cdot X^T \vec{y}$$

$$\Leftrightarrow \boxed{\vec{\beta} = (X^T X)^{-1} \cdot X^T \vec{y}}$$

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# Minimizing the Sum of Squared Errors

Optimality condition:  $\underbrace{X^T}_{(K+1) \times \dots} \underbrace{X \vec{\beta}}_{\dots \times 1} \stackrel{!}{=} \underbrace{X^T \vec{y}}_{(K+1) \times 1} \leftarrow \text{Other ideas to get } \vec{\beta} ??$

How to get the optimal weights  $\vec{\beta}$  ?

If  $X^T X$  has full rank, then the inverse exists and we get:

$$\Leftrightarrow (X^T X)^{-1} \cdot X^T X \vec{\beta} = (X^T X)^{-1} \cdot X^T \vec{y}$$

$$\Leftrightarrow I \cdot \vec{\beta} = (X^T X)^{-1} \cdot X^T \vec{y}$$

$$\Leftrightarrow \vec{\beta} = (X^T X)^{-1} \cdot X^T \vec{y}$$

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# Minimizing the Sum of Squared Errors

Optimality condition:  $\underbrace{X^T}_{(K+1) \times \dots} X \underbrace{\vec{\beta}}_{\dots \times 1} \stackrel{!}{=} \underbrace{X^T \vec{y}}_{(K+1) \times 1} \longleftarrow$  *or solve  $A\vec{x} = \vec{b}$  for  $\vec{x}$*   
*where  $A = X^T X$*   
*and  $\vec{x} = \vec{\beta}$ ,  $\vec{b} = X^T \vec{y}$*

How to get the optimal weights  $\vec{\beta}$  ?

If  $X^T X$  has full rank, then the inverse exists and we get:

$$\Leftrightarrow (X^T X)^{-1} \cdot X^T X \vec{\beta} = (X^T X)^{-1} \cdot X^T \vec{y}$$

$$\Leftrightarrow I \cdot \vec{\beta} = (X^T X)^{-1} \cdot X^T \vec{y}$$

$$\Leftrightarrow \vec{\beta} = (X^T X)^{-1} \cdot X^T \vec{y}$$

# Summary

- Recap I: Cholesky Decomposition
- Recap II: Linear Basis Function Models
- Recap III: Linear Regression & Matrix Algebra

$\mathbf{y}$	$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$
$\mathbf{Ax}$	$\mathbf{A}^T$
$\mathbf{x}^T \mathbf{A}$	$\mathbf{A}$
$\mathbf{x}^T \mathbf{x}$	$2\mathbf{x}$
$\mathbf{x}^T \mathbf{Ax}$	$\mathbf{Ax} + \mathbf{A}^T \mathbf{x}$

$$(\mathbf{A} + \mathbf{B})^T = \mathbf{A}^T + \mathbf{B}^T$$

$$(c \cdot \mathbf{A})^T = c \cdot \mathbf{A}^T$$

$$(\mathbf{A}^T)^T = \mathbf{A}$$

$$(\mathbf{A} \cdot \mathbf{B})^T = \mathbf{B}^T \cdot \mathbf{A}^T$$

$$(\mathbf{A}^{-1})^T = (\mathbf{A}^T)^{-1}$$

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See you next Week!