Maths for ML

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Maths for ML

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Maths for ML

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3. For a scalar s
$$s = s^T$$

Maths for ML

4. Derivative of a scalar s wrt a vector $\boldsymbol{\theta}$

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_N \end{bmatrix}$$

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Linear Functions: Row Vector Times Column Vector

Definition: Setup

Configuration:

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Example: Concrete Example

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{2\times 1}, \quad \boldsymbol{A} = \begin{bmatrix} A_1 & A_2 \end{bmatrix}_{1\times 2}$$

Linear Functions: Row Vector Times Column Vector

Key Points

Matrix Multiplication Result

$$\boldsymbol{A\theta} = A_1\theta_1 + A_2\theta_2$$

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This form appears everywhere in ML:

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- Linear regression: $\boldsymbol{w}^T\boldsymbol{x}$
- Neural networks: $\boldsymbol{w}^T\boldsymbol{h} + b$
- Loss functions: $\boldsymbol{c}^T\boldsymbol{\theta}$

Gradient of Linear Function: Key Result

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Computing the Gradient

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Goal: Find $\frac{\partial \boldsymbol{A\theta}}{\partial \boldsymbol{\theta}}$ where $\boldsymbol{A\theta} = A_1\theta_1 + A_2\theta_2$

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Example: Step-by-Step Calculation

$$\frac{\partial \boldsymbol{A\theta}}{\partial \boldsymbol{\theta}} = \begin{bmatrix} \frac{\partial}{\partial \theta_1}(A_1\theta_1 + A_2\theta_2) \\ \frac{\partial}{\partial \theta_2}(A_1\theta_1 + A_2\theta_2) \end{bmatrix}$$

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$$= \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}_{2\times 1} = \boldsymbol{A}^T$$

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Definition: Intuition

Why $\boldsymbol{A}^T$?

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Definition: Intuition

Why $\boldsymbol{A}^T$? Each component of the gradient equals the coefficient of the corresponding parameter in the linear function.

Quadratic Forms and Their Derivatives

Quadratic Forms: Introduction

Definition: Quadratic Form Derivative Rule

Key Result: For matrix $\boldsymbol{Z}$ of form $\boldsymbol{X}^T\boldsymbol{X}$:

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Starting with:

$$\boldsymbol{X} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad \boldsymbol{X}^T = \begin{bmatrix} a & c \\ b & d \end{bmatrix}$$

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Important: Symmetric Property

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Important: Symmetric Property

Key Observation: $Z_{ij} = Z_{ji} \Rightarrow \boldsymbol{Z}^T = \boldsymbol{Z}$ (symmetric matrix)

Maths for ML

Let

$$\boldsymbol{Z} = \boldsymbol{X}^T\boldsymbol{X} = \begin{bmatrix} e & f \\ f & g \end{bmatrix}_{2\times2}$$

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The term $\boldsymbol{\theta}^T\boldsymbol{Z}\boldsymbol{\theta}$ is a scalar.

Maths for ML

$$\frac{\partial}{\partial \boldsymbol{\theta}} \boldsymbol{\theta}^T \boldsymbol{Z} \boldsymbol{\theta} = \frac{\partial}{\partial \theta} (e\theta_1^2 + 2f\theta_1\theta_2 + g\theta_2^2)$$

Maths for ML

$$
\begin{aligned}
\frac{\partial}{\partial \boldsymbol{\theta}} \boldsymbol{\theta}^T \boldsymbol{Z} \boldsymbol{\theta} &= \frac{\partial}{\partial \theta}(e\theta_1^2 + 2f\theta_1\theta_2 + g\theta_2^2) \\
&= \begin{bmatrix} \frac{\partial}{\partial \theta_1}(e\theta_1^2 + 2f\theta_1\theta_2 + g\theta_2^2) \\ \frac{\partial}{\partial \theta_2}(e\theta_1^2 + 2f\theta_1\theta_2 + g\theta_2^2) \end{bmatrix}
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Matrix Rank and Invertibility

Matrix Rank: Fundamental Concept

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- **Row perspective:** r row vectors, each with c elements

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Two Equivalent Perspectives For an $r \times c$ matrix:

- **Row perspective:** r row vectors, each with c elements
- **Column perspective:** c column vectors, each with r elements

Matrix Rank: Fundamental Concept

Example: Maximum Rank Rules

- If $r < c$: Maximum rank $= r$ (more columns than rows)

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Important: ML Relevance

Why rank matters:

- Determines if matrix is invertible

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Why rank matters:

- Determines if matrix is invertible
- Affects uniqueness of solutions
- Critical for understanding overfitting

Maths for ML: Matrix Rank

- Given a matrix $\boldsymbol{A}$:

$$\begin{bmatrix} 0 & 1 & 2 \\ 1 & 2 & 1 \\ 2 & 7 & 8 \end{bmatrix}$$

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- $r = c = 3$. Thus, rank is $<= 3$

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- Given a matrix $\boldsymbol{A}$:

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- What is the rank?
- $r = c = 3$. Thus, rank is $<= 3$
- Row 3 can be written as: 3 times Row 1 + 2 times Row 1. Thus, Row 3 is linearly dependent on Row 1 and 2. Thus, rank($\boldsymbol{A}$)=2

Maths for ML: Matrix Rank

What is the rank of

$$\boldsymbol{X} = \begin{bmatrix} 1 & 2 & 4 & 4 \\ 3 & 4 & 8 & 0 \end{bmatrix}$$

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What is the rank of

$$\boldsymbol{X} = \begin{bmatrix} 1 & 2 & 4 & 4 \\ 3 & 4 & 8 & 0 \end{bmatrix}$$

Since $\boldsymbol{X}$ has fewer rows than columns, its maximum rank is equal to the maximum number of linearly independent rows. And because neither row is linearly dependent on the other row, the matrix has 2 linearly independent rows; so its rank is 2.

Maths for ML: Matrix Inverse

Suppose $\boldsymbol{A}$ is an $n \times n$ matrix. The inverse of $\boldsymbol{A}$ is another $n \times n$ matrix, denoted $\boldsymbol{A}^{-1}$, that satisfies the following conditions.

$$\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}_n$$

where $\boldsymbol{I}_n$ is the identity matrix.

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Below, with an example, we illustrate the relationship between a matrix and its inverse.

$$\begin{bmatrix} 2 & 1 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 0.8 & -0.2 \\ -0.6 & 0.4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 0.8 & -0.2 \\ -0.6 & 0.2 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

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There are two ways to determine whether the inverse of a square matrix exists.

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A square matrix that has an inverse is said to be nonsingular or invertible; a square matrix that does not have an inverse is said to be singular.
Not every square matrix has an inverse; but if a matrix does have an inverse, it is unique.