

# Maths for ML

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3. For a scalar  $s$

$$s = s^T$$

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## Example: Concrete Example

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

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This form appears everywhere in ML:



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## Important: ML Relevance

This form appears everywhere in ML:

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

# Gradient of Linear Function: Key Result

## Key Points: Computing the Gradient

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

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# Gradient of Linear Function: Key Result

## Important: Fundamental Rule

$$\frac{\partial \mathbf{A}^T \boldsymbol{\theta}}{\partial \boldsymbol{\theta}} = \mathbf{A}$$

**This is one of the most important rules in ML optimization!**

# Quadratic Forms and Their Derivatives

# Quadratic Forms: Introduction

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Starting with:

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

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**Important: Symmetric Property**

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

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Let

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

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

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

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# Matrix Rank and Invertibility



# Matrix Rank: Fundamental Concept

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- If  $r > c$ : Maximum rank =  $c$  (more rows than columns)
- If  $r = c$ : Maximum rank =  $r = c$  (square matrix)



# Maths for ML: Matrix Rank

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- $\text{rank}(\mathbf{A})=2$

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What is the rank of

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

Since  $\mathbf{X}$  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.



# Pop Quiz #1

## Answer this!

What is the rank of a  $3 \times 3$  matrix  $A$  formed by the outer product of two non-zero vectors,  $u$  ( $3 \times 1$ ) and  $v^T$  ( $1 \times 3$ )?

$$A = uv^T = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix}$$

- A) 0
- B) 1
- C) 2
- D) 3

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Answer: **B) 1**

# Maths for ML: Rank of an Outer Product

## Key Points: Matrix Formation

First, let's construct the matrix  $\mathbf{A} = \mathbf{u}\mathbf{v}^T$ :

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# Maths for ML: Rank of an Outer Product

- **Look at the columns:** Each column is just a scalar multiple of the original vector  $\mathbf{u}$ .

$$\text{Column 1} = v_1 \mathbf{u}, \quad \text{Column 2} = v_2 \mathbf{u}, \quad \text{Column 3} = v_3 \mathbf{u}$$

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- **Look at the rows:** Similarly, each row is a scalar multiple of the original vector  $\mathbf{v}^T$ .

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## Important: Conclusion

Since all rows and columns are linearly dependent on a single vector, the maximum number of linearly independent rows (or columns) is one. Therefore, the rank of the matrix is 1.

# Maths for ML: Matrix Inverse

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

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

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



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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.

# Generalizing Derivatives: Gradients and Jacobians

# Derivatives of $\mathbb{R}^n \rightarrow \mathbb{R}$ : The Gradient

## Definition: Recap: Derivative of a Scalar Function

For a function  $f: \mathbb{R}^n \rightarrow \mathbb{R}$  that takes a vector  $\theta \in \mathbb{R}^n$  and returns a scalar, its derivative is the **gradient**.

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$$\nabla f(\theta) = \frac{\partial f}{\partial \theta} = \begin{bmatrix} \frac{\partial f}{\partial \theta_1} \\ \frac{\partial f}{\partial \theta_2} \\ \vdots \\ \frac{\partial f}{\partial \theta_n} \end{bmatrix}_{n \times 1}$$

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**Note:** By convention in ML, the gradient is a column vector.



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**Note:** By convention in ML, the gradient is a column vector.

## Important: Geometric Intuition

The gradient vector  $\nabla f(\theta)$  points in the direction of the **steepest ascent** of the function  $f$  at point  $\theta$ . The magnitude  $\|\nabla f(\theta)\|$  gives the rate of that increase.

From  $\mathbb{R}^n \rightarrow \mathbb{R}$  to  $\mathbb{R}^n \rightarrow \mathbb{R}^m$

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Let  $\mathbf{f} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ . We can think of  $\mathbf{f}$  as a stack of  $m$  scalar-valued functions:

$$\mathbf{f}(\boldsymbol{\theta}) = \begin{bmatrix} f_1(\boldsymbol{\theta}) \\ f_2(\boldsymbol{\theta}) \\ \vdots \\ f_m(\boldsymbol{\theta}) \end{bmatrix}_{m \times 1}$$

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We need to track how **every output** changes with respect to **every input**.

# The Jacobian Matrix

## Definition: The Derivative of a Vector Function

The derivative of  $\mathbf{f}: \mathbb{R}^n \rightarrow \mathbb{R}^m$  is the **Jacobian matrix**  $\mathbf{J}$ , an  $m \times n$  matrix of all first-order partial derivatives.

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**Key Structure:** Row  $i$  of the Jacobian is the transpose of the gradient of the  $i$ -th output function,  $f_i$ .

$$(\mathbf{J})_{[i,:]} = (\nabla f_i(\boldsymbol{\theta}))^T$$



# Jacobian: A Concrete Example

## Example: Let's Compute a Jacobian

Consider  $\mathbf{f}: \mathbb{R}^2 \rightarrow \mathbb{R}^2$  with  $\boldsymbol{\theta} = [\theta_1, \theta_2]^T$ .

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$$\mathbf{J} = \begin{bmatrix} 2\theta_1\theta_2 & \theta_1^2 \\ 5 & \cos(\theta_2) \end{bmatrix}$$