

# Lecture 1

## Basics of Linear Algebra

- Matrix Operations
- Matrix Derivative and Expectations
- Applications and Wrap-Up

# Contents

- Matrix Operations
- Matrix Derivative and Expectations
- Applications and Wrap-Up

# Motivation

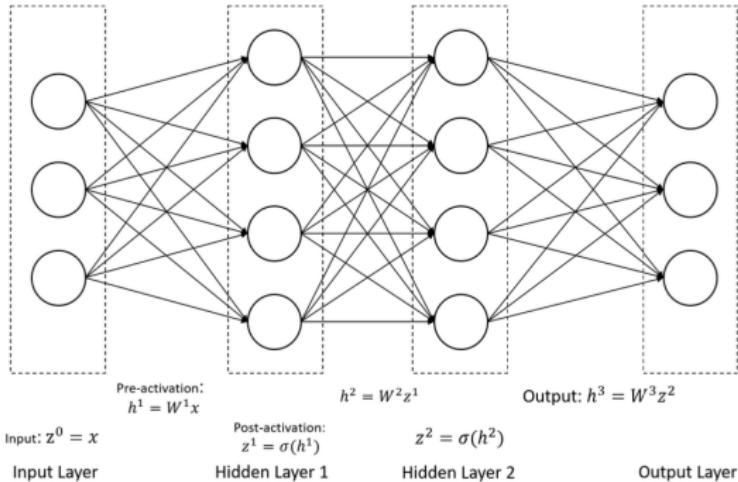


Figure: Example of a 3-layer fully-connected neural network. You should be able to understand its matrix representation.

# What is a Matrix?

Let  $A = (a_{ij})$  be an  $m \times n$  matrix.

- The  $j$ th column of  $A$  is denoted by a column vector  $\mathbf{a}_j$ , i.e.,

$$\mathbf{a}_j = \begin{bmatrix} a_{1j} \\ a_{2j} \\ \vdots \\ a_{mj} \end{bmatrix}$$

- The  $i$ th row of  $A$  is denoted by a row vector  $\vec{\mathbf{a}}_i$ , i.e.,

$$\vec{\mathbf{a}}_i = (a_{i1}, a_{i2}, \dots, a_{in})$$

- Matrix  $A$  can be represented in terms of either its columns and rows:

$$A = [\mathbf{a}_1, \dots, \mathbf{a}_n] = \begin{bmatrix} \vec{\mathbf{a}}_1 \\ \vec{\mathbf{a}}_2 \\ \vdots \\ \vec{\mathbf{a}}_m \end{bmatrix}$$

# Matrix-Vector Multiplication

For an  $m \times n$  matrix  $A$  with the  $i$ th column  $\mathbf{a}_i$ , and a vector  $\mathbf{u} = (u_1, u_2, \dots, u_n)^\top$ , the multiplication of  $A$  and  $\mathbf{u}$  is defined as

$$A\mathbf{u} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + \cdots + u_n\mathbf{a}_n$$

## Example

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 3 & 4 & 5 \end{bmatrix} \begin{bmatrix} 6 \\ -7 \\ 8 \\ -9 \end{bmatrix} = 6 \begin{bmatrix} 1 \\ 2 \end{bmatrix} - 7 \begin{bmatrix} 2 \\ 3 \end{bmatrix} + 8 \begin{bmatrix} 3 \\ 4 \end{bmatrix} - 9 \begin{bmatrix} 4 \\ 5 \end{bmatrix}$$

# Inner Product

- Given a vector  $\mathbf{a} = (a_1, \dots, a_n)^\top$  and a vector  $\mathbf{b} = (b_1, \dots, b_n)^\top$ , following the rule of matrix-vector product, we have

$$\mathbf{a}^\top \mathbf{b} = a_1 b_1 + a_2 b_2 + \cdots + a_n b_n$$

- We call this special vector-vector multiplication the **inner product** (scalar product) of  $\mathbf{a}$  and  $\mathbf{b}$  (denoted by  $\mathbf{a}^\top \mathbf{b}$  or  $\langle \mathbf{a}, \mathbf{b} \rangle$ )
- Properties: Commutative, bilinear
- Application: Cosine similarity,  $\cos \theta = \frac{\mathbf{a}^\top \mathbf{b}}{\|\mathbf{a}\| \|\mathbf{b}\|}$

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## Row Perspective of Multiplication

The matrix-vector multiplication  $A\mathbf{u}$  has a row formula as

$$A\mathbf{u} = \begin{bmatrix} \vec{\mathbf{a}}_1 \mathbf{u} \\ \vec{\mathbf{a}}_2 \mathbf{u} \\ \vdots \\ \vec{\mathbf{a}}_m \mathbf{u} \end{bmatrix}$$

- Consider  $A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 3 & 4 & 5 \end{bmatrix}$  and  $\mathbf{u} = \begin{bmatrix} 6 & -7 & 8 & -9 \end{bmatrix}^\top$ .
- We calculate

$$\vec{\mathbf{a}}_1 \mathbf{u} = 6 \cdot 1 - 7 \cdot 2 + 8 \cdot 3 - 9 \cdot 4 = -20$$

$$\vec{\mathbf{a}}_2 \mathbf{u} = 6 \cdot 2 - 7 \cdot 3 + 8 \cdot 4 - 9 \cdot 5 = -22$$

- We see that  $A\mathbf{u} = \begin{bmatrix} -20 & -22 \end{bmatrix}^\top$

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## Linear Systems as Matrix Equations

Write the following linear systems into compact matrix form:

$$\begin{cases} 2x_1 + x_2 + x_3 = 5 \\ 4x_1 - 6x_2 = -2 \\ -2x_1 + 7x_2 + 2x_3 = 9 \end{cases} \Rightarrow A\mathbf{x} = \mathbf{b}$$

where

$$A = \begin{bmatrix} 2 & 1 & 1 \\ 4 & -6 & 0 \\ -2 & 7 & 2 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 5 \\ -2 \\ 9 \end{bmatrix}$$

## Rank of a Matrix

- The rank of a matrix  $A$  is the number of linearly independent columns
- Equivalently, it is the number of linearly independent rows
- Example:  $A = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}$  has rank 1
- Full rank:  $\text{rank}(A) = \min(m, n)$  for  $A \in \mathbb{R}^{m \times n}$
- Application: Determines solvability of linear systems  $Ax = b$

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# Identity Matrix

- The identity matrix of order  $k$ , denoted by  $I$  or  $I_k$ , is a  $k \times k$  square matrix whose diagonal elements are 1's and whose nondiagonal elements are 0's

$$I = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

- Properties:  $AI = A$  for any compatible matrix  $A$ .

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# Inverse of a Matrix

- Let  $A$  be a  $k \times k$  matrix. The inverse of  $A$ , denoted by  $A^{-1}$ , is another  $k \times k$  matrix such that

$$AA^{-1} = A^{-1}A = I$$

- If the inverse exists, it is unique
- Existence:  $A^{-1}$  exists if and only if  $\det(A) \neq 0$  (or equivalently,  $\text{rank}(A) = k$ )
- For  $2 \times 2$  matrix:

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad A^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

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## Transpose of a Matrix

- Let  $A$  be an  $n \times k$  matrix. The transpose of  $A$ , denoted by  $A^\top$ , is a  $k \times n$  matrix whose columns are the rows of  $A$

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nk} \end{bmatrix} \Rightarrow A^\top = \begin{bmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{12} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & & \vdots \\ a_{1k} & a_{2k} & \cdots & a_{nk} \end{bmatrix}$$

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# Symmetric Matrices

- Let  $A$  be a  $k \times k$  matrix.  $A$  is said to be symmetric if

$$A = A^\top$$

- Examples: Covariance matrices, Hessian matrices
- Properties: Real eigenvalues, orthogonal eigenvectors
- Spectral theorem:  $A = Q\Lambda Q^\top$  where  $Q$  is orthogonal and  $\Lambda$  is diagonal

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# **Idempotent Matrices**

- Let  $A$  be a  $k \times k$  matrix.  $A$  is called idempotent if

$$A = AA$$

- If  $A$  is also symmetric, then  $A$  is called symmetric idempotent
- If  $A$  is symmetric idempotent, then  $I - A$  is also symmetric idempotent
- Example: Projection matrices  $P = X(X^\top X)^{-1}X^\top$

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# Orthonormal Matrices

- Let  $A$  be a  $k \times k$  matrix. If  $A$  is an orthonormal matrix, then

$$A^\top A = I$$

- As a consequence, if  $A$  is an orthonormal matrix, then

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- Properties: Preserves norms and angles ( $\|Ax\| = \|x\|$ )
- Examples: Rotation matrices, permutation matrices

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## Quadratic Forms

- Let  $\mathbf{y}$  be a  $k \times 1$  vector, and let  $A$  be a  $k \times k$  matrix. The function

$$\mathbf{y}^\top A \mathbf{y} = \sum_{i=1}^k \sum_{j=1}^k a_{ij} y_i y_j$$

is called a quadratic form

- Geometric interpretation: Ellipsoids in  $k$ -dimensional space
- Example: Energy in physical systems, Mahalanobis distance

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# Positive Definite and Positive Semidefinite Matrices

Let  $A$  be a  $k \times k$  matrix.

- $A$  is said to be *positive definite* if
  - (a)  $A = A^\top$  ( $A$  is symmetric)
  - (b)  $\mathbf{y}^\top A \mathbf{y} > 0 \quad \forall \mathbf{y} \in \mathbb{R}^k, \mathbf{y} \neq 0$
- $A$  is said to be *positive semidefinite* if:
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  - (c)  $\mathbf{y}^\top A \mathbf{y} \geq 0 \quad \forall \mathbf{y} \in \mathbb{R}^k$
- Tests: Eigenvalues  $> 0$  (positive definite), eigenvalues  $\geq 0$  (positive semidefinite)
- Application: Convex optimization, kernel methods

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## Trace of a Matrix

Let  $A$  be a  $k \times k$  matrix. The *trace* of  $A$ , denoted by  $\text{trace}(A)$  or  $\text{tr}(A)$ , is the sum of the diagonal elements of  $A$ ; thus,

$$\text{trace}(A) = \sum_{i=1}^k a_{ii}$$

### Properties:

1. If  $A$  is an  $m \times n$  matrix and  $B$  is an  $n \times m$  matrix, then

$$\text{trace}(AB) = \text{trace}(BA)$$

2. If the matrices are appropriately conformable, then

$$\text{trace}(ABC) = \text{trace}(CAB)$$

3. If  $A$  and  $B$  are  $k \times k$  matrices and  $a$  and  $b$  are scalars, then

$$\text{trace}(aA + bB) = a\text{trace}(A) + b\text{trace}(B)$$

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## Rank of an Idempotent Matrix

- Let  $A$  be an idempotent matrix. The rank of  $A$  is equal to its trace

$$\text{rank}(A) = \text{trace}(A)$$

- Proof sketch: Use the fact that idempotent matrices are diagonalizable with eigenvalues 0 or 1
- Application: In regression,  $\text{rank}(X) = \text{trace}(H)$  where  $H = X(X^\top X)^{-1}X^\top$  is the hat matrix

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## An Important Identity for a Partitioned Matrix

Let  $\mathbf{X}$  be an  $n \times p$  matrix partitioned such that

$$\mathbf{X} = [\mathbf{X}_1, \mathbf{X}_2]$$

We note that

$$\mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{X} = \mathbf{X}$$

$$\mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top [\mathbf{X}_1 \ \mathbf{X}_2] = \mathbf{X}$$

$$\mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top [\mathbf{X}_1 \ \mathbf{X}_2] = [\mathbf{X}_1 \ \mathbf{X}_2]$$

Consequently,

$$\mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{X}_1 = \mathbf{X}_1 \quad \text{and} \quad \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{X}_2 = \mathbf{X}_2$$

Similarly,

$$\mathbf{X}_1^\top \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top = \mathbf{X}_1^\top \quad \text{and} \quad \mathbf{X}_2^\top \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top = \mathbf{X}_2^\top$$

## Inverse of a Partitioned Matrix

Consider a matrix of the form

$$\mathbf{X}^\top \mathbf{X} = \begin{bmatrix} \mathbf{X}_1^\top \mathbf{X}_1 & \mathbf{X}_1^\top \mathbf{X}_2 \\ \mathbf{X}_2^\top \mathbf{X}_1 & \mathbf{X}_2^\top \mathbf{X}_2 \end{bmatrix}$$

It can be shown that the inverse of this matrix is  $(\mathbf{X}^\top \mathbf{X})^{-1}$  that equals

$$\begin{bmatrix} (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} + (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} \mathbf{X}_1^\top \mathbf{X}_2 G \mathbf{X}_2^\top \mathbf{X}_1 (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} & -(\mathbf{X}_1^\top \mathbf{X}_1)^{-1} \mathbf{X}_1^\top \mathbf{X}_2 G \\ -(\mathbf{X}_1^\top \mathbf{X}_1)^{-1} \mathbf{X}_1^\top \mathbf{X}_2 G & G \end{bmatrix}$$

where

$$\mathbf{H}_1 = \mathbf{X}_1 (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} \mathbf{X}_1^\top \quad \text{and} \quad G = [\mathbf{X}_2^\top (\mathbf{I} - \mathbf{H}_1) \mathbf{X}_2]^{-1}$$

Application: Regression analysis with multiple groups of predictors

# Determinant

- The determinant of a square matrix  $A$ , denoted  $\det(A)$  or  $|A|$ , is a scalar value
- Geometric interpretation: Scaling factor of the linear transformation
- For  $2 \times 2$  matrix:  $\det \begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - bc$
- Properties:
  - $\det(AB) = \det(A) \det(B)$
  - $\det(A^{-1}) = 1/\det(A)$
  - $\det(A^\top) = \det(A)$
- Application: Testing invertibility, change of variables in integration

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# Contents

- Matrix Operations
- Matrix Derivative and Expectations
- Applications and Wrap-Up

# Matrix Derivatives

Let  $\mathbf{A}$  be a  $k \times k$  matrix of constants,  $\mathbf{a}$  be a  $k \times 1$  vector of constants, and  $\mathbf{y}$  be a  $k \times 1$  vector of variables.

1. If  $z = \mathbf{a}^\top \mathbf{y}$ , then

$$\frac{\partial z}{\partial \mathbf{y}} = \frac{\partial(\mathbf{a}^\top \mathbf{y})}{\partial \mathbf{y}} = \mathbf{a}$$

2. If  $z = \mathbf{y}^\top \mathbf{y}$ , then

$$\frac{\partial z}{\partial \mathbf{y}} = \frac{\partial(\mathbf{y}^\top \mathbf{y})}{\partial \mathbf{y}} = 2\mathbf{y}$$

3. If  $z = \mathbf{a}^\top \mathbf{A} \mathbf{y}$ , then

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4. If  $z = \mathbf{y}^\top \mathbf{A} \mathbf{y}$  and  $\mathbf{A}$  is symmetric, then

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## More Derivative Rules

- Application: Gradient descent optimization

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \nabla f(\mathbf{w}_t)$$

where  $\nabla f(\mathbf{w})$  is the gradient of the objective function

- Example: For linear regression with loss  $L(\mathbf{w}) = \|\mathbf{y} - X\mathbf{w}\|^2$ , the gradient is

$$\nabla L(\mathbf{w}) = -2X^\top(\mathbf{y} - X\mathbf{w})$$

- Chain rule for matrix derivatives: If  $z = f(\mathbf{y})$  and  $\mathbf{y} = g(\mathbf{x})$ , then

$$\frac{\partial z}{\partial \mathbf{x}} = \left( \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \right)^\top \frac{\partial z}{\partial \mathbf{y}}$$

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## Expectations of Random Vectors

Let  $A$  be a  $k \times k$  matrix of constants,  $a$  be a  $k \times 1$  vector of constants, and  $y$  be a  $k \times 1$  random vector with mean  $\mu$  and nonsingular variance-covariance matrix  $V$ .

1.  $\mathbb{E}(a^\top y) = a^\top \mu$
2.  $\mathbb{E}(Ay) = A\mu$
3.  $\text{Var}(a^\top y) = a^\top Va$
4.  $\text{Var}(Ay) = AVA^\top$

*Note:* If  $V = \sigma^2 I$ , then  $\text{Var}(Ay) = \sigma^2 AA^\top$

5.  $\mathbb{E}(y^\top Ay) = \text{trace}(AV) + \mu^\top A\mu$

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# Applications of Matrix Expectations

- Portfolio variance: For portfolio returns  $\mathbf{r}$  with weights  $\mathbf{w}$ ,

$$\text{Var}(\mathbf{w}^\top \mathbf{r}) = \mathbf{w}^\top \Sigma \mathbf{w}$$

where  $\Sigma$  is the covariance matrix of returns

- Risk estimation: For quadratic loss functions
- Signal processing: For estimating power in transformed signals
- Econometrics: In GMM and other estimation methods

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# Applications in AI

- Neural networks: Weight matrices and activation functions

$$\mathbf{h}^{(l)} = f(W^{(l)}\mathbf{h}^{(l-1)} + \mathbf{b}^{(l)})$$

- Principal Component Analysis (PCA): Eigendecomposition of covariance matrix

$$\Sigma = Q\Lambda Q^\top$$

- Linear regression: Least squares solution

$$\hat{\beta} = (X^\top X)^{-1} X^\top y$$

- Support Vector Machines: Quadratic optimization with linear constraints

## Further Reading

- Strang, G. (2016). *Introduction to Linear Algebra*
- Boyd, S. & Vandenberghe, L. (2018). *Introduction to Applied Linear Algebra*
- MIT OpenCourseWare: Linear Algebra

Next lecture: Derivative of Neural Network Functions