### Definition, Properties, and Derivatives of Matrix Traces

A Class for Undergraduate Students

@Southern University of Science and Technology

Xinyu Chen

March 31, 2023



### **Class Targets**

Throughout this class, you will:

- Understanding some basic concepts (e.g., norms, traces, and derivatives)
- connecting them with linear algebra and machine learning
- Using matrix norms and traces in matrix computations (very useful!)



#### Vector & Matrix

#### Notation:

• On the vector  ${m x} \in \mathbb{R}^n$  of length n

$$oldsymbol{x} = (x_1, x_2, \cdots, x_n)^{ op} \quad ext{or} \quad oldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

whose *i*-th entry is  $x_i$ ,  $i \in [1, n]$ .

### Vector & Matrix

#### Notation:

• On the vector  $oldsymbol{x} \in \mathbb{R}^n$  of length n

$$m{x} = (x_1, x_2, \cdots, x_n)^{ op} \quad ext{or} \quad m{x} = egin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

whose *i*-th entry is  $x_i$ ,  $i \in [1, n]$ .

ullet On the matrix  $oldsymbol{X} \in \mathbb{R}^{m imes n}$  with m rows and n columns

$$m{X} = egin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \ x_{21} & x_{22} & \cdots & x_{2n} \ dots & dots & dots & dots \ x_{m1} & x_{m2} & \cdots & x_{mn} \end{bmatrix}$$

whose (i, j)-th entry is  $x_{ij}, i \in [1, m], j \in [1, n]$ .

#### **Vector Norms**

Derivatives

A number of concepts to mention, e.g.,  $\ell_0$ -norm,  $\ell_1$ -norm, and  $\ell_2$ -norm.

**Definition.** For any vector  $\mathbf{x} \in \mathbb{R}^n$ , the  $\ell_2$ -norm of  $\mathbf{x}$  is given by

$$\|\boldsymbol{x}\|_{2} = \sqrt{x_{1}^{2} + x_{2}^{2} + \dots + x_{n}^{2}} = \sqrt{\sum_{i=1}^{n} x_{i}^{2}}$$

where  $x_i, \forall i \in [1, n]$  is the *i*-th entry of  $\boldsymbol{x}$ .

### **Vector Norms**

Derivatives

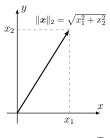
A number of concepts to mention, e.g.,  $\ell_0$ -norm,  $\ell_1$ -norm, and  $\ell_2$ -norm.

**Definition.** For any vector  $\mathbf{x} \in \mathbb{R}^n$ , the  $\ell_2$ -norm of  $\mathbf{x}$  is given by

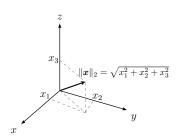
$$\|\boldsymbol{x}\|_{2} = \sqrt{x_{1}^{2} + x_{2}^{2} + \dots + x_{n}^{2}} = \sqrt{\sum_{i=1}^{n} x_{i}^{2}}$$

where  $x_i, \forall i \in [1, n]$  is the *i*-th entry of  $\boldsymbol{x}$ .

Intuitive examples:



On 
$$\boldsymbol{x} = (x_1, x_2)^{\top}$$



On 
$$x = (x_1, x_2, x_3)^{\top}$$

### Inner Product

• Basics: For any  $\boldsymbol{x} = (x_1, x_2)^{\top}$  and  $\boldsymbol{y} = (y_1, y_2)^{\top}$ , the angle  $\theta$  can be computed by

$$\cos \theta = \frac{x_1 y_1 + x_2 y_2}{\sqrt{x_1^2 + x_2^2} \sqrt{y_1^2 + y_2^2}}$$



- in which
  - $\circ$   $\ell_2$ -norm:

$$\|\boldsymbol{x}\|_2 = \sqrt{x_1^2 + x_2^2}$$
  $\|\boldsymbol{y}\|_2 = \sqrt{y_1^2 + y_2^2}$ 

o inner product:

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \boldsymbol{x}^{\top} \boldsymbol{y} = x_1 y_1 + x_2 y_2$$

It leads to

$$\cos \theta = \frac{\langle \boldsymbol{x}, \boldsymbol{y} \rangle}{\|\boldsymbol{x}\|_2 \cdot \|\boldsymbol{y}\|_2}$$

#### Inner Product

Derivatives

**Definition.** For any vectors  $x, y \in \mathbb{R}^n$ , the inner product is given by

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \boldsymbol{x}^{\top} \boldsymbol{y} = \sum_{i=1}^{n} x_i y_i$$

**Example.** Given  $\boldsymbol{x} = (1, 2, 3, 4)^{\top}$  and  $\boldsymbol{y} = (2, -1, 3, 0)^{\top}$ , write down the inner product  $\langle x, y \rangle$ .

In this case,

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \boldsymbol{x}^{\top} \boldsymbol{y} = 1 \times 2 + 2 \times (-1) + 3 \times 3 + 4 \times 0 = 9$$

0000000

### **Inner Product**

• **Definition.** For any matrices  $X, Y \in \mathbb{R}^{m \times n}$ , the inner product is

$$\langle \boldsymbol{X}, \boldsymbol{Y} \rangle = \sum_{i=1}^{m} \sum_{j=1}^{n} x_{ij} y_{ij}$$

**Example.** Given 
$$X = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$
 and  $Y = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$ , write down the

inner product  $\langle \boldsymbol{X}, \boldsymbol{Y} \rangle$ .

In this case,

$$\langle X, Y \rangle = 2 \times 2 + 1 \times (-1) + 1 \times (-1) + 2 \times 2 + 1 \times (-1) + 3 \times 2 = 11$$

#### Frobenius Norm

• **Definition.** For any matrix  $X \in \mathbb{R}^{m \times n}$ , the Frobenius norm of X is given by

$$\|X\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n x_{ij}^2}$$

where  $x_{ij}$ ,  $\forall i \in [1, m], j \in [1, n]$  is the (i, j)-th entry of X.

**Example.** Given  $X = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix}$ , write down the Frobenius norm of X.

$$\|\boldsymbol{X}\|_F = \sqrt{2^2 + 1^2 + 1^2 + 1^2 + 2^2 + 1^2 + 3^2} = \sqrt{21}$$

#### Frobenius Norm

• Connection with  $\ell_2$ -norm:

$$\|m{X}\|_F = \sqrt{\sum_{j=1}^n \sum_{i=1}^m x_{ij}^2} = \sqrt{\sum_{j=1}^n \|m{x}_j\|_2^2}$$

with the column vectors  $\boldsymbol{x}_j \in \mathbb{R}^m, \, j \in [1,n]$  such that

$$oldsymbol{X} = egin{bmatrix} ert & ert & ert & ert \ oldsymbol{x}_1 & oldsymbol{x}_2 & \cdots & oldsymbol{x}_n \ ert & ert & ert & ert \end{bmatrix} \in \mathbb{R}^{m imes n}$$

#### **Definition of Matrix Trace**

**Definition.** For any square matrix  $X \in \mathbb{R}^{n \times n}$ , the matrix trace (denoted by  $tr(\cdot)$ ) is the sum of diagonal entries, i.e.,

$$\operatorname{tr}(\boldsymbol{X}) = \sum_{i=1}^{n} \underbrace{x_{ii}}_{\mathsf{diagonal}}$$

where  $x_{ii}$ ,  $\forall i \in [1, n]$  is the (i, i)-th entry of X. Thus,  $\operatorname{tr}(X) = \operatorname{tr}(X^{\top})$ .

**Example.** Given  $X = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix}$ , write down the matrix trace of X.

$$tr(X) = 2 + 2 + 3 = 7$$

Summary

## **Property:** tr(X + Y) = tr(X) + tr(Y)

ullet Property. For any square matrices  $m{X}, m{Y} \in \mathbb{R}^{n imes n}$ , it always holds that  $\mathrm{tr}(m{X} + m{Y}) = \mathrm{tr}(m{X}) + \mathrm{tr}(m{Y})$ 

**Example.** Given 
$$X = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$
 and  $Y = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$ , write down  $\operatorname{tr}(X + Y)$ .

In this case,

$$\mathbf{X} + \mathbf{Y} = \begin{bmatrix} 2+2 & 1-1 & 1+0 \\ 1-1 & 2+2 & 1-1 \\ 0+0 & 0-1 & 3+2 \end{bmatrix} = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 4 & 0 \\ 0 & -1 & 5 \end{bmatrix}$$

Thus,  $\operatorname{tr}(\boldsymbol{X} + \boldsymbol{Y}) = 4 + 4 + 5 = 13$ . Note that  $\operatorname{tr}(\boldsymbol{X}) = 7$  and  $\operatorname{tr}(\boldsymbol{Y}) = 6$ , it shows that  $\operatorname{tr}(\boldsymbol{X} + \boldsymbol{Y}) = \operatorname{tr}(\boldsymbol{X}) + \operatorname{tr}(\boldsymbol{Y}) = 13$ .

• Variant. For any  $\alpha, \beta \in \mathbb{R}$ , we have

$$\operatorname{tr}(\alpha \boldsymbol{X} + \beta \boldsymbol{Y}) = \alpha \operatorname{tr}(\boldsymbol{X}) + \beta \operatorname{tr}(\boldsymbol{Y})$$

## **Property:** tr(XY) = tr(YX)

• Property. For any matrices  $X \in \mathbb{R}^{m \times n}$  and  $Y \in \mathbb{R}^{n \times m}$ , it always holds that

$$\operatorname{tr}(\boldsymbol{X}\boldsymbol{Y}) = \operatorname{tr}(\boldsymbol{Y}\boldsymbol{X})$$

Proof.

$$tr(XY) = [XY]_{11} + [XY]_{22} + \dots + [XY]_{mm}$$

$$= \underbrace{x_{11}y_{11} + x_{12}y_{21} + \dots + x_{1n}y_{n1}}_{\text{the first row of } X \text{ times the first column of } Y$$

$$+ x_{21}y_{12} + x_{22}y_{22} + \dots + x_{2n}y_{n2}$$

$$+ \dots + x_{m1}y_{1m} + x_{m2}y_{2m} + \dots + x_{mn}y_{nm}$$

## **Property:** tr(XY) = tr(YX)

• **Property.** For any matrices  $X \in \mathbb{R}^{m \times n}$  and  $Y \in \mathbb{R}^{n \times m}$ , it always holds that

$$\operatorname{tr}(\boldsymbol{X}\boldsymbol{Y}) = \operatorname{tr}(\boldsymbol{Y}\boldsymbol{X})$$

• Proof.

$$\operatorname{tr}(\boldsymbol{X}\boldsymbol{Y}) = [\boldsymbol{X}\boldsymbol{Y}]_{11} + [\boldsymbol{X}\boldsymbol{Y}]_{22} + \dots + [\boldsymbol{X}\boldsymbol{Y}]_{mm}$$

$$= \underbrace{x_{11}y_{11} + x_{12}y_{21} + \dots + x_{1n}y_{n1}}_{\text{the first row of }\boldsymbol{X} \text{ times the first column of }\boldsymbol{Y}$$

$$+ x_{21}y_{12} + x_{22}y_{22} + \dots + x_{2n}y_{n2}$$

$$+ \dots + x_{m1}y_{1m} + x_{m2}y_{2m} + \dots + x_{mn}y_{nm}$$

$$= x_{11}y_{11} + x_{12}y_{21} + \dots + x_{1n}y_{n1}$$

$$+ x_{21}y_{12} + x_{22}y_{22} + \dots + x_{2n}y_{n2}$$

$$+ \dots + x_{m1}y_{1m} + x_{m2}y_{2m} + \dots + x_{mn}y_{nm}$$

## Property: tr(XY) = tr(YX)

• Property. For any matrices  $X \in \mathbb{R}^{m \times n}$  and  $Y \in \mathbb{R}^{n \times m}$ , it always holds that

$$tr(XY) = tr(YX)$$

Proof.

**Basics** 

$$\operatorname{tr}(\boldsymbol{X}\boldsymbol{Y}) = [\boldsymbol{X}\boldsymbol{Y}]_{11} + [\boldsymbol{X}\boldsymbol{Y}]_{22} + \dots + [\boldsymbol{X}\boldsymbol{Y}]_{mm}$$

$$= \frac{x_{11}y_{11} + x_{12}y_{21} + \dots + x_{1n}y_{n1}}{\operatorname{the first row of } \boldsymbol{X} \text{ times the first column of } \boldsymbol{Y}$$

$$+ x_{21}y_{12} + x_{22}y_{22} + \dots + x_{2n}y_{n2}$$

$$+ \dots + x_{m1}y_{1m} + x_{m2}y_{2m} + \dots + x_{mn}y_{nm}$$

$$= x_{11}y_{11} + x_{12}y_{21} + \dots + x_{1n}y_{n1}$$

$$+ x_{21}y_{12} + x_{22}y_{22} + \dots + x_{2n}y_{n2}$$

$$+ \dots + x_{m1}y_{1m} + x_{m2}y_{2m} + \dots + x_{mn}y_{nm}$$

$$= \frac{y_{11}x_{11} + y_{12}x_{21} + \dots + y_{1m}x_{m1}}{\operatorname{the first row of } \boldsymbol{Y} \text{ times the first column of } \boldsymbol{X}$$

$$+ y_{21}x_{12} + y_{22}x_{22} + \dots + y_{2m}x_{m2}$$

$$+ \dots + y_{n1}x_{1n} + \dots + y_{n2}x_{2n} + \dots + y_{nm}x_{mn}$$

$$= [\boldsymbol{Y}\boldsymbol{X}]_{11} + [\boldsymbol{Y}\boldsymbol{X}]_{22} + \dots + [\boldsymbol{Y}\boldsymbol{X}]_{nn} = \operatorname{tr}(\boldsymbol{Y}\boldsymbol{X})$$

## Property: tr(XY) = tr(YX)

**Example.** Given 
$$\boldsymbol{X} = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$
 and  $\boldsymbol{Y} = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$ , write down  $\operatorname{tr}(\boldsymbol{X}\boldsymbol{Y})$  and  $\operatorname{tr}(\boldsymbol{Y}\boldsymbol{X})$ , respectively.

In this case,

$$\mathbf{XY} = \begin{bmatrix} 3 & -1 & 1 \\ 0 & 2 & 0 \\ 0 & -3 & 6 \end{bmatrix} \qquad \mathbf{YX} = \begin{bmatrix} 3 & 0 & 1 \\ 0 & 3 & -2 \\ -1 & -2 & 5 \end{bmatrix}$$

Thus,

$$tr(XY) = 3 + 2 + 6 = 11$$
  $tr(YX) = 3 + 3 + 5 = 11$ 

# Property: $\|\boldsymbol{X}\|_F^2 = \operatorname{tr}(\boldsymbol{X}^{\top}\boldsymbol{X})$

• **Property.** For any matrix  $X \in \mathbb{R}^{m \times n}$ , it always holds that

$$\|\boldsymbol{X}\|_F^2 = \operatorname{tr}(\boldsymbol{X}^{\top}\boldsymbol{X})$$

• Proof.

$$\operatorname{tr}(\boldsymbol{X}^{\top}\boldsymbol{X}) = [\boldsymbol{X}^{\top}\boldsymbol{X}]_{11} + [\boldsymbol{X}^{\top}\boldsymbol{X}]_{22} + \dots + [\boldsymbol{X}^{\top}\boldsymbol{X}]_{nn}$$

$$= x_{11}^{2} + x_{21}^{2} + \dots + x_{m1}^{2}$$

$$+ x_{12}^{2} + x_{22}^{2} + \dots + x_{m2}^{2}$$

$$+ \dots + x_{1n}^{2} + x_{2n}^{2} + \dots + x_{mn}^{2}$$

$$= \sum_{i=1}^{m} x_{i1}^{2} + \sum_{i=1}^{m} x_{i2}^{2} + \dots + \sum_{i=1}^{m} x_{in}^{2}$$

$$= \sum_{i=1}^{m} \sum_{j=1}^{n} x_{ij}^{2}$$

$$= \|\boldsymbol{X}\|_{F}^{2}$$

# Property: $\langle \boldsymbol{X}, \boldsymbol{Y} \rangle = \operatorname{tr}(\boldsymbol{X}^{\top} \boldsymbol{Y})$

• **Property.** For any matrices  $X, Y \in \mathbb{R}^{m \times n}$ , it always holds that

$$\langle \boldsymbol{X}, \boldsymbol{Y} \rangle = \operatorname{tr}(\boldsymbol{X}^{\top} \boldsymbol{Y})$$

Proof.

$$\operatorname{tr}(\boldsymbol{X}^{\top}\boldsymbol{Y}) = [\boldsymbol{X}^{\top}\boldsymbol{Y}]_{11} + [\boldsymbol{X}^{\top}\boldsymbol{Y}]_{22} + \dots + [\boldsymbol{X}^{\top}\boldsymbol{Y}]_{nn}$$

$$= x_{11}y_{11} + x_{21}y_{21} + \dots + x_{m1}y_{m1}$$

$$+ x_{12}y_{12} + x_{22}y_{22} + \dots + x_{m2}y_{m2}$$

$$+ \dots + x_{1n}y_{1n} + x_{2n}y_{2n} + \dots + x_{mn}y_{mn}$$

$$= \langle \boldsymbol{x}_1, \boldsymbol{y}_1 \rangle + \langle \boldsymbol{x}_2, \boldsymbol{y}_2 \rangle + \dots + \langle \boldsymbol{x}_n, \boldsymbol{y}_n \rangle$$

$$= \langle \boldsymbol{X}, \boldsymbol{Y} \rangle$$

where  $x_i, y_i \in \mathbb{R}^m$ ,  $\forall i \in [1, n]$  are the *i*-th column vectors of X and Y, respectively.

# Property: $\langle \boldsymbol{X}, \boldsymbol{Y} \rangle = \operatorname{tr}(\boldsymbol{X}^{\top} \boldsymbol{Y})$

**Example.** Given 
$$X = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$
 and  $Y = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$ , write down

Recall that

$$\langle X, Y \rangle = 2 \times 2 + 1 \times (-1) + 1 \times (-1) + 2 \times 2 + 1 \times (-1) + 3 \times 2 = 11$$

For the matrix,

$$\boldsymbol{X}^{\top}\boldsymbol{Y} = \begin{bmatrix} 3 & 0 & -1 \\ 0 & 3 & -2 \\ 1 & -2 & 5 \end{bmatrix}$$

we have  $tr(X^{T}Y) = 3 + 3 + 5 = 11$ .

 $\langle \boldsymbol{X}, \boldsymbol{Y} \rangle$  and  $\operatorname{tr}(\boldsymbol{X}^{\top} \boldsymbol{Y})$ , respectively.

### **Derivatives**

#### A quick revisit!

ullet Derivative. Given a scalar function f(x) of the single variable x, the derivative is defined by

$$\frac{\mathrm{d} f(x)}{\mathrm{d} x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} = \lim_{\Delta x \to 0} \frac{\Delta f}{\Delta x}$$

#### **Derivatives**

A quick revisit!

• **Derivative.** Given a scalar function f(x) of the single variable x, the derivative is defined by

$$\frac{\mathrm{d}\,f(x)}{\mathrm{d}\,x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} = \lim_{\Delta x \to 0} \frac{\Delta f}{\Delta x}$$

• Partial derivatives. Given a scalar function f(x,y) of two variables x,y, the partial derivatives are defined by

$$\begin{cases} \frac{\partial f(x,y)}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x, y)}{\Delta x} \\ \frac{\partial f(x,y)}{\partial y} = \lim_{\Delta x \to 0} \frac{f(x,y + \Delta y)}{\Delta y} \end{cases}$$

### **Derivatives**

**Example.** Given  $f(x) = ||x||_2^2$ , write down the derivative  $\frac{\mathrm{d} f(x)}{\mathrm{d} x}$ .

First, notice that the function  $f(\boldsymbol{x})$  can be written as

$$f(\mathbf{x}) = f(x_1, x_2, \dots, x_n) = x_1^2 + x_2^2 + \dots + x_n^2$$

Hence, the partial derivatives of  $f(x_1, x_2, \dots, x_n)$  with respect to  $x_1, x_2, \dots, x_n$  are

$$\frac{\partial f(x_1, x_2, \dots, x_n)}{\partial x_1} = 2x_1$$

$$\frac{\partial f(x_1, x_2, \dots, x_n)}{\partial x_2} = 2x_2$$

$$\vdots$$

$$\frac{\partial f(x_1, x_2, \dots, x_n)}{\partial x_2} = 2x_2$$

$$\vdots$$

$$\frac{\partial f(x_1, x_2, \dots, x_n)}{\partial x_n} = 2x_n$$

$$\frac{\partial f(x_1, x_2, \dots, x_n)}{\partial x_n} = 2x_n$$

$$\frac{\partial f(x_1, x_2, \dots, x_n)}{\partial x_n} = 2x_n$$

### **Derivative of** f(X) = tr(X)

Derivatives

0000000

- Function. For any square matrix  $X \in \mathbb{R}^{n \times n}$ , what is the derivative of  $f(\boldsymbol{X}) = \operatorname{tr}(\boldsymbol{X})$ ?
- ullet Derivative. Since  $f(oldsymbol{X}) = \sum^n x_{ii}$ , we have

$$\frac{\mathrm{d}f(\boldsymbol{X})}{\mathrm{d}\boldsymbol{X}} = \begin{bmatrix}
\frac{\partial f(\boldsymbol{X})}{\partial x_{11}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{12}} & \dots & \frac{\partial f(\boldsymbol{X})}{\partial x_{1n}} \\
\frac{\partial f(\boldsymbol{X})}{\partial x_{21}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{22}} & \dots & \frac{\partial f(\boldsymbol{X})}{\partial x_{2n}} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial f(\boldsymbol{X})}{\partial x_{n1}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{n2}} & \dots & \frac{\partial f(\boldsymbol{X})}{\partial x_{nn}}
\end{bmatrix}$$

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

Summary

## Derivative of f(X) = tr(AX)

Derivatives

- Function. For any matrices  $A \in \mathbb{R}^{m \times n}$  and  $X \in \mathbb{R}^{n \times m}$ , what is the derivative of f(X) = tr(AX)?
- Derivative. Since

$$f(\boldsymbol{X}) = \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} x_{ji}$$

Hence, the partial derivative of f(X) with respect to the entry  $x_{ii}$  is given by

$$\frac{\partial f(\boldsymbol{X})}{\partial x_{ji}} = a_{ij}$$

As a result, we have

$$\frac{\mathrm{d}f(\boldsymbol{X})}{\mathrm{d}\boldsymbol{X}} = \begin{bmatrix} \frac{\partial f(\boldsymbol{X})}{\partial x_{11}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{12}} & \cdots & \frac{\partial f(\boldsymbol{X})}{\partial x_{1m}} \\ \frac{\partial f(\boldsymbol{X})}{\partial f(\boldsymbol{X})} & \frac{\partial f(\boldsymbol{X})}{\partial x_{22}} & \cdots & \frac{\partial f(\boldsymbol{X})}{\partial x_{2m}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(\boldsymbol{X})}{\partial x_{n1}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{n2}} & \cdots & \frac{\partial f(\boldsymbol{X})}{\partial x_{nm}} \end{bmatrix} = \boldsymbol{A}^{\top}$$

• By the way, what is the derivative of f(X) = tr(XA)? How about  $f(\boldsymbol{X}) = \operatorname{tr}(\boldsymbol{A}^{\top} \boldsymbol{X}^{\top})$ ?

Summary

### **Derivative of** f(X) = tr(AXB)

- Function. For any matrices  $A \in \mathbb{R}^{m \times n}$ ,  $X \in \mathbb{R}^{n \times d}$ , and  $B \in \mathbb{R}^{d \times m}$ , what is the derivative of f(X) = tr(AXB)?
- Derivative. Since

$$f(\mathbf{X}) = \sum_{i=1}^{m} [\mathbf{A} \mathbf{X} \mathbf{B}]_{i,i} = \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} [\mathbf{X} \mathbf{B}]_{j,i} = \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} \sum_{k=1}^{d} x_{jk} b_{ki}$$

Hence, the partial derivative of f(X) with respect to the entry  $x_{ik}$  is given by

$$\frac{\partial f(\boldsymbol{X})}{\partial x_{jk}} = \sum_{i=1}^{m} a_{ij} b_{ki} = [\boldsymbol{A}^{\top} \boldsymbol{B}^{\top}]_{j,k}$$

As a result, we have

$$\frac{\mathrm{d} f(\boldsymbol{X})}{\mathrm{d} \boldsymbol{X}} = \begin{bmatrix} \frac{\partial f(\boldsymbol{X})}{\partial x_{11}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{12}} & \cdots & \frac{\partial f(\boldsymbol{X})}{\partial x_{1d}} \\ \frac{\partial f(\boldsymbol{X})}{\partial x_{21}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{22}} & \cdots & \frac{\partial f(\boldsymbol{X})}{\partial x_{2d}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(\boldsymbol{X})}{\partial x_{r+1}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{r+2}} & \cdots & \frac{\partial f(\boldsymbol{X})}{\partial x_{r}} \end{bmatrix} = \boldsymbol{A}^{\mathsf{T}} \boldsymbol{B}^{\mathsf{T}}$$

# Derivative of $f(\boldsymbol{X}) = \operatorname{tr}(\boldsymbol{X}^{\top} \boldsymbol{A} \boldsymbol{X})$

- Function. For any matrices  $A, X \in \mathbb{R}^{n \times n}$ , what is the derivative of  $f(X) = \operatorname{tr}(X^{\top}AX)$ ?
- Derivative.

$$\frac{\mathrm{d} f(X)}{\mathrm{d} X} = \frac{\mathrm{d} \operatorname{tr}(X^{\top} B)}{\mathrm{d} X} + \frac{\mathrm{d} \operatorname{tr}(CX)}{\mathrm{d} X}$$
$$= \frac{\mathrm{d} \operatorname{tr}(B^{\top} X)}{\mathrm{d} X} + \frac{\mathrm{d} \operatorname{tr}(CX)}{\mathrm{d} X}$$
$$= B + C^{\top}$$
$$= AX + AX^{\top}$$

where  $oldsymbol{B} riangleq oldsymbol{A} oldsymbol{X}$  and  $oldsymbol{C} riangleq oldsymbol{X}^ op oldsymbol{A}$ .

### **Derivative of** f(X) = tr(AXBXC)

- Function. For any matrices  $A \in \mathbb{R}^{m \times n}$ ,  $X \in \mathbb{R}^{n \times d}$ ,  $B \in \mathbb{R}^{d \times n}$ , and  $C \in \mathbb{R}^{d \times m}$ , what is the derivative of  $f(X) = \operatorname{tr}(AXBXC)$ ?
- Derivative.

$$\frac{\mathrm{d} f(X)}{\mathrm{d} X} = \frac{\mathrm{d} \operatorname{tr}(AXD)}{\mathrm{d} X} + \frac{\mathrm{d} \operatorname{tr}(EXC)}{\mathrm{d} X}$$
$$= A^{\top} D^{\top} + E^{\top} C^{\top}$$
$$= A^{\top} C^{\top} X^{\top} B^{\top} + B^{\top} X^{\top} A^{\top} C^{\top}$$

where  $D \triangleq BXC$  and  $E \triangleq AXB$ .

## Derivative of $f(X) = ||AX||_F^2$

- Function. For any matrices  $A \in \mathbb{R}^{m \times n}$  and  $X \in \mathbb{R}^{n \times d}$ , what is the derivative of  $f(X) = ||AX||_E^2$ ?
- Derivative. Since

$$f(\boldsymbol{X}) = \operatorname{tr}(\boldsymbol{X}^{\top} \boldsymbol{A}^{\top} \boldsymbol{A} \boldsymbol{X})$$

Hence, we have

$$\frac{\mathrm{d} f(\mathbf{X})}{\mathrm{d} \mathbf{X}} = \frac{\mathrm{d} \operatorname{tr}(\mathbf{B} \mathbf{X})}{\mathrm{d} \mathbf{X}} + \frac{\mathrm{d} \operatorname{tr}(\mathbf{X}^{\top} \mathbf{B}^{\top})}{\mathbf{X}}$$
$$= \frac{\mathrm{d} \operatorname{tr}(\mathbf{B} \mathbf{X})}{\mathrm{d} \mathbf{X}} + \frac{\mathrm{d} \operatorname{tr}(\mathbf{B} \mathbf{X})}{\mathrm{d} \mathbf{X}}$$
$$= 2\mathbf{B}^{\top}$$
$$= 2\mathbf{A}^{\top} \mathbf{A} \mathbf{X}$$

where  $B \triangleq X^{\top} A^{\top} A$ 

### **Orthogonal Procrustes Problem (Optional)**

#### • Orthogonal Procrustes problem:

For any  $Q \in \mathbb{R}^{m \times r}$ ,  $m \ge r$ , the solution to

$$\min_{m{F}} \ \|m{F} - m{Q}\|_F^2$$

s.t. 
$$\mathbf{F}^{\top} \mathbf{F} = \mathbf{I}_r$$
 orthogonal

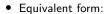
is

$$F := UV^{\top}$$

where

$$oldsymbol{Q} = oldsymbol{U} oldsymbol{\Sigma} oldsymbol{V}^{ op}$$

singular value decomposition



$$\|\boldsymbol{F} - \boldsymbol{Q}\|_F^2 = \operatorname{tr}(\boldsymbol{F}^\top \boldsymbol{F} - \boldsymbol{F}^\top \boldsymbol{Q} - \boldsymbol{Q}^\top \boldsymbol{F} + \underline{\boldsymbol{Q}}^\top \boldsymbol{Q}) = -2\operatorname{tr}(\boldsymbol{F}^\top \boldsymbol{Q}) + \operatorname{const.}$$

$$\Longrightarrow \!\! \boldsymbol{F} = : \underset{\boldsymbol{F}^{\top}\boldsymbol{F} = \boldsymbol{I}_r}{\arg\min} \ \|\boldsymbol{F} - \boldsymbol{Q}\|_F^2 = \underset{\boldsymbol{F}^{\top}\boldsymbol{F} = \boldsymbol{I}_r}{\arg\max} \ \operatorname{tr}(\boldsymbol{F}^{\top}\boldsymbol{Q})$$



### A Quick Look

#### Content:

- Vector structure,  $\ell_2$ -norm
- Matrix structure. Frobenius norm
- Inner product
- Definition, properties, and derivatives of matrix trace (including a lot of examples)

#### For your need!

- Slides: https://xinychen.github.io/slides/matrix\_trace.pdf
- E-book:

https://xinychen.github.io/books/spatiotemporal\_low\_rank\_models.pdf

#### Reference material:

• The matrix cookbook:

https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf

### Special thanks to

Zhanhong Cheng (McGill University)

for providing feedback and suggestions when correcting the slides.

- Fuqiang Liu (McGill University)

• Sheng Liu (UESTC)

# Thanks for your attention!

Any Questions?

#### About me:

Homepage: https://xinychen.github.io

• How to reach me: chenxy346@gmail.com

