Definition, Properties, and Derivatives of Matrix Traces

A Class for Undergraduate Students

Xinyu Chen

March 31, 2024

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:

Basics

•000000

ullet 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 , $i \in [n]$.¹

 $^{^1}$ The set of integers, $\{1,2,\ldots,n\}$, is represented by $[n],\,n\in\mathbb{Z}^+.$

Vector & Matrix

Notation:

Basics

•000000

ullet 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 , $i \in [n]$.¹

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

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

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

¹The set of integers, $\{1,2,\ldots,n\}$, is represented by $[n],\,n\in\mathbb{Z}^+$.

Vector Norms

A number of concepts to mention, e.g., ℓ_0 -norm, ℓ_1 -norm, and ℓ_2 -norm.

Definition. For any vector $\mathbf{x} \in \mathbb{R}^n$, the ℓ_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 $x_i, \forall i \in [n]$ is the *i*-th entry of \boldsymbol{x} .

Vector Norms

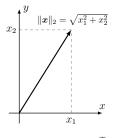
A number of concepts to mention, e.g., ℓ_0 -norm, ℓ_1 -norm, and ℓ_2 -norm.

Definition. For any vector $\mathbf{x} \in \mathbb{R}^n$, the ℓ_2 -norm of \mathbf{x} is given by

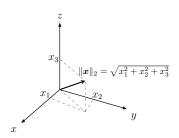
$$\|x\|_2 = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2} = \sqrt{\sum_{i=1}^n x_i^2}$$

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

Intuitive examples:



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



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

Inner Product

• Basics: For any $\boldsymbol{x} = (x_1, x_2)^{\top}$ and $\boldsymbol{y} = (y_1, y_2)^{\top}$, the angle θ 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 ℓ_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

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

where $x_{ij}, \forall i \in [m], j \in [n]$ is the (i, j)-th entry of \boldsymbol{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 ℓ_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 $\boldsymbol{x}_j \in \mathbb{R}^m, j \in [n]$ such that

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

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 $x_{ii}, \forall i \in [n]$ 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.

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

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

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

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

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

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

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

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

In this case,

tr(XY) and tr(YX), respectively.

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

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

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

• 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 $x_i, y_i \in \mathbb{R}^m$, $\forall i \in [n]$ 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

Derivatives

•0000000

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

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

Derivatives

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

First, notice that the function f(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 $f(x_1, x_2, \ldots, x_n)$ with respect to x_1, x_2, \ldots, x_n are

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

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

$$\vdots$$

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

$$\vdots$$

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

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

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

Summary

Derivative of f(X) = tr(X)

- 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)

Derivatives

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

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

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

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

Derivative of f(X) = tr(AXBXC)

Derivatives

00000000

- 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

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

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

Orthogonal Procrustes Problem (Optional)

• Orthogonal Procrustes problem:

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

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

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

is

$$oldsymbol{F} := oldsymbol{U}oldsymbol{V}^{ op}$$

where

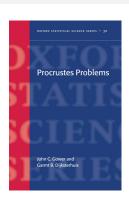
$$oldsymbol{Q} = oldsymbol{U} oldsymbol{\Sigma} oldsymbol{V}^{ op}$$

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, ℓ_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)
- Benzheng Li (UESTC)

 Formula (M. Gill III)
- Fuqiang Liu (McGill University)Sheng Liu (UESTC)

for providing feedback and suggestions.

Thanks for your attention!

Any Questions?

About me:

- Homepage: https://xinychen.github.io
- How to reach me: chenxy346@gmail.com