Definition, Properties, and Derivatives of Matrix Traces

A Class for Undergraduate Students
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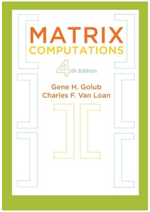
Class Targets

Throughout this class, you will:

- Understanding some basic concepts and connect them with linear algebra and machine learning
- Using matrix norms and traces in matrix computations (very useful!)



Vector & Matrix

Notation:

- On the vector $\boldsymbol{x} \in \mathbb{R}^n$ of length n

$$\boldsymbol{x} = (x_1, x_2, \cdots, x_n)^\top \quad \text{or} \quad \boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

- On the matrix $\boldsymbol{X} \in \mathbb{R}^{m \times n}$ with m rows and n columns

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

Vector Norms

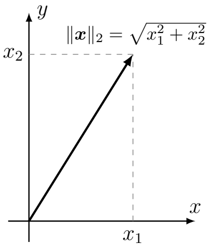
A number of concepts to mention, e.g., ℓ_0-norm, ℓ_1-norm, and ℓ_2-norm.

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

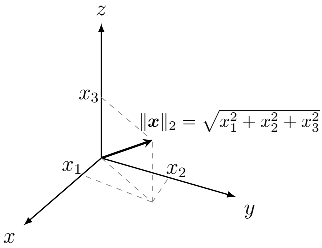
$$\|\boldsymbol{x}\|_2 = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} = \sqrt{\sum_{i=1}^{n} x_i^2}$$

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

Inner Product

- Revisit ...

Frobenius Norm

- **Definition.** For any matrix $\boldsymbol{X} \in \mathbb{R}^{m \times n}$, the Frobenius norm of $\boldsymbol{X}$ 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 $\boldsymbol{X} = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 0 & 0 & 3 \end{bmatrix}$, write down the Frobenius norm of $\boldsymbol{X}$.

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

Frobenius Norm

- Connection with ℓ_2-norm:

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

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

$$\boldsymbol{X} = \begin{bmatrix} | & | & & | \\ \boldsymbol{x}_1 & \boldsymbol{x}_2 & \cdots & \boldsymbol{x}_n \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{m\times n}$$

Definition of Matrix Trace

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

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

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

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

$$\operatorname{tr}(\boldsymbol{X}) = 2 + 2 + 3 = 7$$

Property: $\mathrm{tr}(\boldsymbol{X}+\boldsymbol{Y}) = \mathrm{tr}(\boldsymbol{X}) + \mathrm{tr}(\boldsymbol{Y})$

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

$$\mathrm{tr}(\boldsymbol{X}+\boldsymbol{Y}) = \mathrm{tr}(\boldsymbol{X}) + \mathrm{tr}(\boldsymbol{Y})$$

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 $\mathrm{tr}(\boldsymbol{X}+\boldsymbol{Y})$.

In this case,

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

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

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

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

Property: $\mathrm{tr}(\boldsymbol{X}\boldsymbol{Y}) = \mathrm{tr}(\boldsymbol{Y}\boldsymbol{X})$

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

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

- **Proof.**

$$\begin{aligned}
\mathrm{tr}(\boldsymbol{X}\boldsymbol{Y}) =& (\boldsymbol{X}\boldsymbol{Y})_{11} + (\boldsymbol{X}\boldsymbol{Y})_{22} + \cdots + (\boldsymbol{X}\boldsymbol{Y})_{mm} \\
=& x_{11}y_{11} + x_{12}y_{21} + \cdots + x_{1n}y_{n1} \\
& + x_{21}y_{12} + x_{22}y_{22} + \cdots + x_{2n}y_{n2} \\
& + \cdots + x_{m1}y_{1m} + x_{m2}y_{2m} + \cdots + x_{mn}y_{nm} \\
=& y_{11}x_{11} + y_{12}x_{21} + \cdots + y_{1m}x_{m1} \\
& + y_{21}x_{12} + y_{22}x_{22} + \cdots + y_{2m}x_{m2} \\
& + \cdots + y_{n1}x_{1n} + \cdots + y_{n2}x_{2n} + \cdots + y_{nm}x_{mn} \\
=& (\boldsymbol{Y}\boldsymbol{X})_{11} + (\boldsymbol{Y}\boldsymbol{X})_{22} + \cdots + (\boldsymbol{Y}\boldsymbol{X})_{nn} \\
=& \mathrm{tr}(\boldsymbol{Y}\boldsymbol{X})
\end{aligned}$$

Property: $\mathrm{tr}(\boldsymbol{XY}) = \mathrm{tr}(\boldsymbol{YX})$

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 $\mathrm{tr}(\boldsymbol{XY})$ and $\mathrm{tr}(\boldsymbol{YX})$, respectively.

In this case,

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

Thus,

$$\mathrm{tr}(\boldsymbol{XY}) = 3 + 2 + 6 = 11 \qquad \mathrm{tr}(\boldsymbol{YX}) = 3 + 3 + 5 = 11$$

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

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

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

- **Proof.**

$$\begin{aligned}
\mathrm{tr}(\boldsymbol{X}^\top \boldsymbol{X}) =& (\boldsymbol{X}^\top \boldsymbol{X})_{11} + (\boldsymbol{X}^\top \boldsymbol{X})_{22} + \cdots + (\boldsymbol{X}^\top \boldsymbol{X})_{nn} \\
=& x_{11}^2 + x_{21}^2 + \cdots + x_{m1}^2 \\
& + x_{12}^2 + x_{22}^2 + \cdots + x_{m2}^2 \\
& + \cdots + x_{1n}^2 + x_{2n}^2 + \cdots + x_{mn}^2 \\
=& \sum_{i=1}^m x_{i1}^2 + \sum_{i=1}^m x_{i2}^2 + \cdots + \sum_{i=1}^m x_{in}^2 \\
=& \sum_{i=1}^m \sum_{j=1}^n x_{ij}^2 \\
=& \|\boldsymbol{X}\|_F^2
\end{aligned}$$

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

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

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

- **Proof.**

$$\begin{aligned} \mathrm{tr}(\boldsymbol{X}^\top \boldsymbol{Y}) =& (\boldsymbol{X}^\top \boldsymbol{Y})_{11} + (\boldsymbol{X}^\top \boldsymbol{Y})_{22} + \cdots + (\boldsymbol{X}^\top \boldsymbol{Y})_{nn} \\ = & \end{aligned}$$

Derivatives

Orthogonal Procrustes Problem

- **Orthogonal Procrustes problem**: For any $\boldsymbol{Q} \in \mathbb{R}^{m \times r}$, $m \geq r$, the solution to

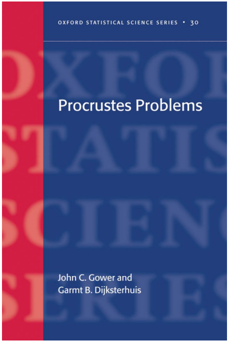
$$\min_{\boldsymbol{F}} \ \|\boldsymbol{F} - \boldsymbol{Q}\|_F^2 \quad \text{s.t.} \ \underbrace{\boldsymbol{F}^\top \boldsymbol{F} = \boldsymbol{I}_r}_{\text{orthogonal}}$$

is

$$\boldsymbol{F} := \boldsymbol{U}\boldsymbol{V}^\top$$

where

$$\underbrace{\boldsymbol{Q} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^\top}_{\text{singular value decomposition}}$$



- Equivalent form:

$$\|\boldsymbol{F} - \boldsymbol{Q}\|_F^2 = \mathrm{tr}(\underbrace{\boldsymbol{F}^\top \boldsymbol{F}}_{=\boldsymbol{I}_r} - \boldsymbol{F}^\top \boldsymbol{Q} - \boldsymbol{Q}^\top \boldsymbol{F} + \underbrace{\boldsymbol{Q}^\top \boldsymbol{Q}}_{\text{const.}}) = -2\,\mathrm{tr}(\boldsymbol{F}^\top \boldsymbol{Q}) + \text{const.}$$

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

A Quick Look

Content:

- Vector structure, ℓ_2-norm
- Matrix structure, Frobenius norm
- 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

Thanks for your attention!

Any Questions?

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