Definition, Properties, and Derivatives of Matrix Traces

A Class for Undergraduate Students
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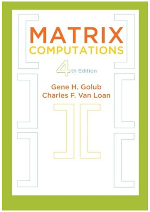
Class Targets

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

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

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

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

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

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

Vector Norms

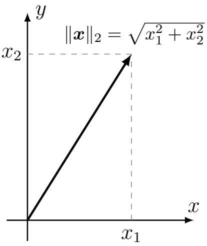
A number of concepts to mention, e.g., ℓ_0-norm, ℓ_1-norm, and ℓ_2-norm.

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

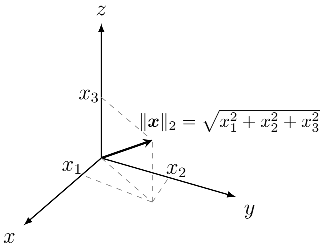
$$\|\boldsymbol{x}\|_2 = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} = \sqrt{\sum_{i=1}^{n} x_i^2}$$

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

- Intuitive examples:



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

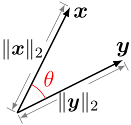


On $\boldsymbol{x} = (x_1, x_2, x_3)^\top$

Inner Product

- 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
  - ℓ_2-norm:

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

  - 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

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

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

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

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

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

In this case,

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

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.,

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

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

- **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
$$\mathrm{tr}(\boldsymbol{XY}) = \mathrm{tr}(\boldsymbol{YX})$$
- **Proof.**

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

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

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 $\mathrm{tr}(\boldsymbol{X}\boldsymbol{Y})$ and $\mathrm{tr}(\boldsymbol{Y}\boldsymbol{X})$, respectively.

In this case,

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

Thus,

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

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

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

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

- **Proof.**

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

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.**

$$\begin{aligned}
\mathrm{tr}(\boldsymbol{X}^\top \boldsymbol{Y}) =& [\boldsymbol{X}^\top \boldsymbol{Y}]_{11} + [\boldsymbol{X}^\top \boldsymbol{Y}]_{22} + \cdots + [\boldsymbol{X}^\top \boldsymbol{Y}]_{nn} \\
=& x_{11}y_{11} + x_{21}y_{21} + \cdots + x_{m1}y_{m1} \\
& + x_{12}y_{12} + x_{22}y_{22} + \cdots + x_{m2}y_{m2} \\
& + \cdots + x_{1n}y_{1n} + x_{2n}y_{2n} + \cdots + x_{mn}y_{mn} \\
=& \langle \boldsymbol{x}_1, \boldsymbol{y}_1 \rangle + \langle \boldsymbol{x}_2, \boldsymbol{y}_2 \rangle + \cdots + \langle \boldsymbol{x}_n, \boldsymbol{y}_n \rangle \\
=& \langle \boldsymbol{X}, \boldsymbol{Y} \rangle
\end{aligned}$$

where $\boldsymbol{x}_i, \boldsymbol{y}_i \in \mathbb{R}^m, \forall i \in [n]$ are the i-th column vectors of $\boldsymbol{X}$ and $\boldsymbol{Y}$, respectively.

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

$$\begin{cases} \dfrac{\partial f(x,y)}{\partial x} = \lim\limits_{\Delta x \to 0} \dfrac{f(x + \Delta x, y)}{\Delta x} \\ \dfrac{\partial f(x,y)}{\partial y} = \lim\limits_{\Delta x \to 0} \dfrac{f(x, y + \Delta y)}{\Delta y} \end{cases}$$

Derivatives

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

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

$$f(\boldsymbol{x}) = f(x_1, x_2, \ldots, x_n) = x_1^2 + x_2^2 + \cdots + x_n^2$$

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

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

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

$$\vdots$$

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

$$\Longrightarrow \quad \frac{\mathrm{d}\, f(\boldsymbol{x})}{\mathrm{d}\, \boldsymbol{x}} = \begin{bmatrix} \frac{\partial f(x_1, x_2, \ldots, x_n)}{\partial x_1} \\ \frac{\partial f(x_1, x_2, \ldots, x_n)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x_1, x_2, \ldots, x_n)}{\partial x_n} \end{bmatrix} = \begin{bmatrix} 2x_1 \\ 2x_2 \\ \vdots \\ 2x_n \end{bmatrix} = 2\boldsymbol{x}$$

Derivative of $f(\boldsymbol{X}) = \operatorname{tr}(\boldsymbol{X})$

- **Function.** For any square matrix $\boldsymbol{X} \in \mathbb{R}^{n \times n}$, what is the derivative of $f(\boldsymbol{X}) = \operatorname{tr}(\boldsymbol{X})$?
- **Derivative.** Since $f(\boldsymbol{X}) = \sum_{i=1}^{n} x_{ii}$, we have

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

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

Derivative of $f(\boldsymbol{X}) = \mathrm{tr}(\boldsymbol{A}\boldsymbol{X})$

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

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

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

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

As a result, we have

$$\frac{\mathrm{d}\, f(\boldsymbol{X})}{\mathrm{d}\,\boldsymbol{X}} = \begin{bmatrix} \frac{\partial f(\boldsymbol{X})}{\partial x_{11}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{12}} & \cdots & \frac{\partial f(\boldsymbol{X})}{\partial x_{1m}} \\ \frac{\partial f(\boldsymbol{X})}{\partial x_{21}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{22}} & \cdots & \frac{\partial f(\boldsymbol{X})}{\partial x_{2m}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(\boldsymbol{X})}{\partial x_{n1}} & \frac{\partial f(\boldsymbol{X})}{\partial x_{n2}} & \cdots & \frac{\partial f(\boldsymbol{X})}{\partial x_{nm}} \end{bmatrix} = \boldsymbol{A}^\top$$

Derivative of $f(\boldsymbol{X}) = \mathrm{tr}(\boldsymbol{A}\boldsymbol{X}\boldsymbol{B})$

Derivative of $f(\boldsymbol{X}) = \operatorname{tr}(\boldsymbol{A}\boldsymbol{X}\boldsymbol{B}\boldsymbol{X}\boldsymbol{C})$

Derivative of $f(\boldsymbol{X}) = \|\boldsymbol{A}\boldsymbol{X}\|_F^2$

Orthogonal Procrustes Problem

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

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

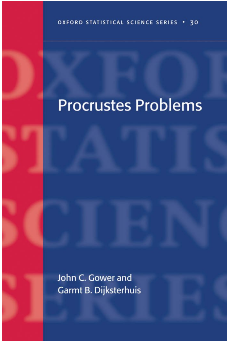
$$\text{s.t.} \ \underbrace{\boldsymbol{F}^\top \boldsymbol{F} = \boldsymbol{I}_r}_{\text{orthogonal}}$$

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:

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

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

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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