Linear Algebra
Matrices and Vectors. First Introduction, Basic Operations.

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MDS FCS HSE

Matrix

> **ℹ Definition**
>
> A **matrix** is an ordered array of numbers arranged in n rows and m columns.
>
> $$A_{n \times m} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{bmatrix}$$

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- We usually denote it as $A_{n \times m}$ or, to emphasize the nature of numbers in the matrix, we write $A \in \mathbb{R}^{n \times m}$.
- If $n = m$, the matrix is called *square*; if $n \neq m$, it's called *rectangular*

Basic operations: transpose

> **i** Definition
>
> **Transpose** of a matrix is an operation where rows and columns are swapped. If $A \in \mathbb{R}^{n \times m}$, then $B = A^T \in \mathbb{R}^{m \times n}$, where $b_{ij} = a_{ji}$

$$
\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} \xrightarrow{A^T} \begin{bmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \\ a_{13} & a_{23} \end{bmatrix}
$$

$$A_{2 \times 3} \qquad\qquad B_{3 \times 2} = A^T$$

-

> **i** Definition
>
> **Matrix addition** is only possible for matrices of the same size. The result is obtained by adding corresponding elements. If $A, B \in \mathbb{R}^{n \times m}$, then $C = A + B$, where $c_{ij} = a_{ij} + b_{ij}$

Example:

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} + \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} = \begin{bmatrix} 1+5 & 2+6 \\ 3+7 & 4+8 \end{bmatrix} = \begin{bmatrix} 6 & 8 \\ 10 & 12 \end{bmatrix}$$

Basic operations: scalar multiplication

-

> **i** Definition
>
> **Scalar multiplication** - each element of the matrix is multiplied by the given number. If $A \in \mathbb{R}^{n \times m}$ and $\alpha \in \mathbb{R}$, then $C = \alpha A$, where $c_{ij} = \alpha \cdot a_{ij}$

Example:

$$3 \cdot \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} 3 \cdot 1 & 3 \cdot 2 \\ 3 \cdot 3 & 3 \cdot 4 \end{bmatrix} = \begin{bmatrix} 3 & 6 \\ 9 & 12 \end{bmatrix}$$

Another example - Linear combination:

$$2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + 3 \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} + \begin{bmatrix} 3 & 3 \\ 3 & 3 \end{bmatrix} = \begin{bmatrix} 5 & 3 \\ 3 & 5 \end{bmatrix}$$

Vector

In the simplest representation, we treat a **vector** as a special case of a matrix:

Column vector

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n \times 1}$$

Dimension: $n \times 1$ (matrix with one column)

Row vector

$$\mathbf{y}^T = \begin{bmatrix} y_1 & y_2 & \cdots & y_m \end{bmatrix} \in \mathbb{R}^{1 \times m}$$

Dimension: $1 \times m$ (matrix with one row)

Notation

- **Vectors:** usually denoted by lowercase letters x, v or $\mathbf{u}$

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- **By default:** vector is considered a **column vector**
- **Transpose:** $\mathbf{x}^\top$ converts column to row

Matrix-by-vector multiplication (matvec)

Standard approach

$$y_1 = a_{11}x_1 + a_{12}x_2 + \cdots + a_{1,m-1}x_{m-1} + a_{1m}x_m$$

$$y_j = \sum_{k=1}^{m} a_{jk}x_k$$

Matrix-by-vector multiplication (matvec)

Computational complexity and a brief look at parallel computing

Recall the general formula:

$$y_j = \sum_{k=1}^{m} a_{jk} x_k, \quad j = 1, 2, \dots, n$$

Operations analysis:

- For computing one element y_j: m multiplications (each $a_{jk} \cdot x_k$), $m-1$ additions (summing m products)
- For the entire vector $\mathbf{y}$ (n elements): $n \cdot (2m-1)$ total operations.

Time complexity:

- For square matrix $n \times n$: $\mathcal{O}(2n^2 - n) = \mathcal{O}(n^2)$
- For rectangular matrix $n \times m$: $\mathcal{O}(nm)$

> 💡 Natural parallelism
>
> Computing each element y_j is **independent** of other elements!

- **Row-wise parallelization:** each processor computes its own y_j

Guru approach

$$
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & a_{14} \\
a_{21} & a_{22} & a_{23} & a_{24} \\
a_{31} & a_{32} & a_{33} & a_{34}
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4
\end{bmatrix}
=
\begin{bmatrix}
y_1 \\
y_2 \\
y_3
\end{bmatrix}
$$

$$A \qquad\qquad \mathbf{x} \qquad\qquad \mathbf{y}$$

Matrix-by-vector multiplication (matvec)

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a_{11} & a_{12} & a_{13} & a_{14} \\
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\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4
\end{bmatrix}
=
\begin{bmatrix}
y_1 \\
y_2 \\
y_3
\end{bmatrix}
$$

$$A \qquad\qquad \mathbf{x} \qquad\qquad \mathbf{y}$$

$$y_1 = a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4$$

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Guru approach

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

$$A \qquad\qquad \mathbf{x} \qquad\qquad \mathbf{y}$$

$$y_1 = a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4$$
$$y_2 = a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + a_{24}x_4$$

Matrix-by-vector multiplication (matvec)

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$$y_1 = a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4$$
$$y_2 = a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + a_{24}x_4$$
$$y_3 = a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + a_{34}x_4$$

Matrix-by-vector multiplication (matvec)

Guru approach

$$
\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}
$$

$$
A \qquad \mathbf{x} \qquad \mathbf{y}
$$

$$
\mathbf{y} = x_1 \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \end{bmatrix} + x_2 \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \end{bmatrix} + x_3 \begin{bmatrix} a_{13} \\ a_{23} \\ a_{33} \end{bmatrix} + x_4 \begin{bmatrix} a_{14} \\ a_{24} \\ a_{34} \end{bmatrix}
$$

Matrix-by-vector product

Visual comparison

$$\begin{bmatrix} 3 & 1 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 7 \\ 8 \end{bmatrix}$$

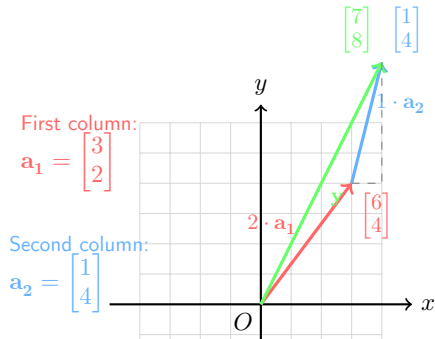$$A \qquad \mathbf{x} \qquad \mathbf{y}$$

Traditional View: Row-wise

Calculations:

- $y_1 = 3 \cdot 2 + 1 \cdot 1 = 7$
- $y_2 = 2 \cdot 2 + 4 \cdot 1 = 8$

Guru View: Column Linear Combination

Linear combination:

Matrix-by-matrix multiplication (matmul, General Matrix Multiplication - GEMM)

Standard approach

$$
\begin{bmatrix}
a_{11} & a_{12} & \cdots & a_{1k} \\
\vdots & \vdots & \ddots & \vdots \\
a_{i1} & a_{i2} & \cdots & a_{ik} \\
\vdots & \vdots & \ddots & \vdots \\
a_{n1} & a_{n2} & \cdots & a_{nk}
\end{bmatrix}
\begin{bmatrix}
b_{11} & \cdots & b_{1j} & \cdots & b_{1m} \\
b_{21} & \cdots & b_{2j} & \cdots & b_{2m} \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
b_{k1} & \cdots & b_{kj} & \cdots & b_{km}
\end{bmatrix}
=
\begin{bmatrix}
c_{11} & \cdots & c_{1j} & \cdots & c_{1m} \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
c_{i1} & \cdots & c_{ij} & \cdots & c_{im} \\
\vdots & \ddots & \vdots & \ddots & \vdots \\
c_{n1} & \cdots & c_{nj} & \cdots & c_{nm}
\end{bmatrix}
$$

i-th row

j-th column

A B C

$$c_{ij} = a_{i1} \cdot b_{1j} + a_{i2} \cdot b_{2j} + \cdots + a_{ik} \cdot b_{kj}$$

$$c_{ij} = \sum_{l=1}^{k} a_{il} b_{lj}$$

Matrix multiplication (matmul, General Matrix Multiplication - GEMM)

Column-wise approach

$$
\begin{bmatrix}
a_{11} & a_{12} & \cdots & a_{1k} \\
\vdots & \vdots & \ddots & \vdots \\
a_{i1} & a_{i2} & \cdots & a_{ik} \\
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b_{k1} & b_{k2} & b_{k3} & \cdots & b_{km}
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=
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\vdots & \vdots & \vdots & \ddots & \vdots \\
c_{n1} & c_{n2} & c_{n3} & \cdots & c_{nm}
\end{bmatrix}
$$

$$A \qquad\qquad B \qquad\qquad C$$

Each column of $C = A\times$ corresponding column of B

$$\boxed{\mathbf{C_j} = A\mathbf{B_j}, \quad j = 1, 2, \ldots, m}$$

Properties of matrix multiplication

1. **Associativity:**

$$(AB)C = A(BC)$$

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  2. **Distributivity:**

$$A(B + C) = AB + AC$$
$$(A + B)C = AC + BC$$

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1. **Associativity:**

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$$A(B + C) = AB + AC$$
$$(A + B)C = AC + BC$$

3. **Scalar multiplication:**

$$\alpha(AB) = (\alpha A)B = A(\alpha B)$$

Important limitations

4. **Non-commutativity:**

$$AB \neq BA \quad \text{(in general)}$$

Example: For 2×2 matrices:

$$\begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 2 \\ 1 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 1 & 3 \end{bmatrix}$$

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$$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 1 & 3 \end{bmatrix}$$

5. **Transpose of product:**

$$(AB)^T = B^T A^T$$

> **i** Уведомление
>
> Note the **reversed order** of matrices when transposing!

Matrix multiplication (matmul, General Matrix Multiplication - GEMM)
Computational complexity and parallelization

Recall the general formula:

$$c_{ij} = \sum_{l=1}^{k} a_{il}b_{lj}, \quad i = 1, 2, ..., n, \quad j = 1, 2, ..., m$$

Operations analysis for matrices $A_{n \times k}$ and $B_{k \times m}$:
- For computing one element c_{ij}: k multiplications, $k-1$ additions
- Total number of operations: $n \times m \times (2k-1)$

Time complexity:
- For square matrices $n \times n$: $\mathcal{O}(2n^3 - n^2) = \mathcal{O}(n^3)$
- For rectangular matrices: $\mathcal{O}(nmk)$

💡 Natural parallelism

- **By elements:** each c_{ij} is computed independently

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- **By rows:** each processor handles its rows of matrix A

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- **By rows:** each processor handles its rows of matrix A
- **By columns:** each processor handles its columns of matrix B
- **Block approach:** dividing matrices into blocks for efficient cache usage

Example. Simple but important idea about matrix computations.

Suppose you have the following expression

$$b = A_1 A_2 A_3 x,$$

where $A_1, A_2, A_3 \in \mathbb{R}^{3 \times 3}$ are random square dense (fully filled with numbers) matrices, and $x \in \mathbb{R}^3$ is a vector. You need to compute b.

Which approach is best to use?

1. $A_1 A_2 A_3 x$ (left to right)
2. $(A_1 (A_2 (A_3 x)))$ (right to left)
3. It doesn't matter
4. The results of the first two options will not be the same.

Check the attached .ipynb file in the repository.