	Maths	Chemistry
A	90	80
B	80	95

$\begin{pmatrix} 90 & 80 \\ 80 & 95 \end{pmatrix}$ 2×2 matrix.

Topic 8. Matrices

Matrices

We can store data as a series of rows and columns. Arranging data in this way is called a matrix.

EXAMPLE: $\underbrace{\begin{pmatrix} 1 & 9 & -13 \\ 20 & 5 & -6 \end{pmatrix}}_{\text{3 columns}}\Big\}$ 2 rows

$a_{11} = 1$. $a_{12} = 9$. a_{ij} i-th row j-th column

In the example, we had 2 rows and 3 columns. This is a 2×3 matrix.

In general, a matrix has dimension (size), $m \times n$, if it has m rows and n columns.

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & & \\ a_{m1} & \vdots & \vdots & \cdots & a_{mn} \end{pmatrix}$$

If $m = n$ (same no. rows as columns), then the matrix is called square.

EXAMPLE: $A = \begin{pmatrix} 3 & -1 & 7 \\ 2 & 4 & 6 \\ 0 & 1 & -2 \end{pmatrix} \rightarrow$ this is a 3×3 matrix, and is square .

Extra notation: If all the elements of a matrix, A, are real numbers and A has dimension $m \times n$, then we say $A \in \mathbb{R}^{(m \times n)}$.

A vector is a matrix: Column vector: $\underline{u} = \underbrace{\begin{pmatrix} 0 \\ 1 \\ 2 \\ 3 \end{pmatrix}}_{4\times 1}$, row vector: $\underline{v} = \underbrace{(5, 6, 7)}_{1\times 3}$.

Matrix operations

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_1+b_1 \\ a_2+b_2 \end{pmatrix}$$

Addition (subtraction)

EXAMPLE: $A = \underbrace{\begin{pmatrix} 3 & 1 \\ 0 & -2 \end{pmatrix}}_{2\times 2}, B = \underbrace{\begin{pmatrix} 1 & 3 \\ 3 & 1 \end{pmatrix}}_{2\times 2}$.

$$A+B = \begin{pmatrix} 3+1 & 1+3 \\ 0+3 & -2+1 \end{pmatrix} = \underbrace{\begin{pmatrix} 4 & 4 \\ 3 & -1 \end{pmatrix}}_{2\times 2}$$

$$A-B = \begin{pmatrix} 3-1 & 1-3 \\ 0-3 & -2-1 \end{pmatrix} = \underbrace{\begin{pmatrix} 2 & -2 \\ -3 & -3 \end{pmatrix}}_{2\times 2}$$

Note: We can only add/subtract matrices of the same size. And the resulting matrix will always be the same size as the one's we started with.

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} + \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix} = \begin{pmatrix} 1+1 & 2+2 & ?+3 \\ 3+4 & 4+5 & ?+6 \end{pmatrix}$$ × we can't do it.

Multiplication by a constant

EXAMPLE: $3A = 3\begin{pmatrix} 3 & 1 \\ 0 & -2 \end{pmatrix}$ $\quad k\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} ka_1 \\ ka_2 \end{pmatrix}$

$$= \begin{pmatrix} 3\times 3 & 3\times 1 \\ 3\times 0 & 3\times(-2) \end{pmatrix}$$

$$= \begin{pmatrix} 9 & 3 \\ 0 & -6 \end{pmatrix}$$

Multiplication

We first consider two vectors being multiplied (row and column vector)

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 \end{pmatrix}, B = \begin{pmatrix} 5 \\ 6 \\ 7 \\ 8 \end{pmatrix}.$$

1×4 4×1

pairwise multiply elements and sum them up:

① 1-st elements of A × 1-st element of B: $1\times 5 = 5$.
2-nd ... of A × 2-nd ... B: $2\times 6 = 12$.
3rd ... A × 3rd ... B: $3\times 7 = 21$
4th ... A × 4th ... B: $4\times 8 = 32$.

②: $5+12+21+32 = 70$.

$A\times B = 70$.

For general matrices, we repeat this process for all pairs of rows and columns.

EXAMPLE: $A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$, $B = \begin{pmatrix} 5 & 6 \\ 7 & 8 \end{pmatrix}$. Find AB.

1-st row of A × 1-st column of B

$$A\times B = \begin{pmatrix} 1\times 5 + 2\times 7 & 1\times 6 + 2\times 8 \\ 3\times 5 + 4\times 7 & 3\times 6 + 4\times 8 \end{pmatrix}$$

→ 1-st row of A × 2nd column of B

→ 2-nd row of A × 2-nd colum of B.

2-nd row of A × 1st colum of B

$$= \begin{pmatrix} 19 & 22 \\ 43 & 50 \end{pmatrix}$$

$\neq$

$$B\times A = \begin{pmatrix} 5 & 6 \\ 7 & 8 \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} = \begin{pmatrix} 5\times 1 + 6\times 3 & 5\times 2 + 6\times 4 \\ 7\times 1 + 8\times 3 & 7\times 2 + 8\times 4 \end{pmatrix}$$

$$= \begin{pmatrix} 23 & 34 \\ 31 & 46 \end{pmatrix}$$

$AB \neq BA$.

order is important!

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1r} \\ \vdots & \vdots & & \vdots \end{pmatrix} \begin{pmatrix} b_{11} & \cdots \\ b_{21} & \cdots \\ \vdots & \\ b_{\ell 1} & \cdots \end{pmatrix} = \begin{pmatrix} a_{11} \times b_{11} + a_{12} \times b_{21} \cdots + a_{1r} \times b_{\ell 1} & \cdots \\ \vdots & \vdots \end{pmatrix}$$

$r = \ell.$

When can we multiply matrices?

We can only multiply two matrices if the lead matrix (matrix on the left of the multiplication) has the same no. of columns as the no. of rows in the lag matrix (matrix on the right).

$$\underset{m \times n}{A} \times \underset{n \times k}{B} = AB \in \mathbb{R}^{m \times k}.$$

match.

Powers of matrices:

$A^2 = AA, A^3 = A^2A = AAA, \ldots, A^n = \underbrace{AAA\cdots A}_{\text{n times A.}}$

Note: $A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$, $A^2 = AA = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \neq \begin{pmatrix} 1^2 & 2^2 \\ 3^2 & 4^2 \end{pmatrix}$

2×2 square.

Not always possible to calculate the power of a matrix.

$B = \begin{pmatrix} 1 & 2 \\ 3 & 6 \\ 5 & 6 \end{pmatrix} \in \mathbb{R}^{3\times 2}$

$\underset{3\times 2}{B} \times \underset{3\times 2}{B}$ ×.

not match.

Properties of multiplication

$(AB)C = A(BC)$

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

Other operations

Transpose: this interchanges rows and columns of a matrix. $\top$

EXAMPLE: $A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}, A^\top = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix}, B = \begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{pmatrix}, B^\top = \begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}.$

$(A^\top)^\top = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$

Things to note:

or $a_{ij} = a_{ji}$

$\left(A^\top\right)^\top = A$ (for all matrices A). If $A^\top = A$, we call A symmetric.

$\begin{pmatrix} 1 & 2 \\ 2 & 3 \end{pmatrix}^\top = \begin{pmatrix} 1 & 2 \\ 2 & 3 \end{pmatrix}$

$(AB)^\top = B^\top A^\top, \quad (A+B)^\top = A^\top + B^\top$

Δ

$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 5 & 4 \\ 3 & 4 & 6 \end{pmatrix}$

Row and column vectors:

$$C = \underbrace{\begin{pmatrix} 0 \\ 1 \\ 2 \\ 3 \end{pmatrix}}_{4\times 1}, C^\top = \underbrace{\begin{pmatrix} 0 & 1 & 2 & 3 \end{pmatrix}}_{1\times 4}$$

Types of matrices and terminology

Lead diagonal: values going from top left to bottom right (usually only for square).

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix} \qquad Tr(A) = 1+5+9 = 15.$$

Trace: trace of a matrix is the sum of the elements in the lead diagonal, denoted by Tr(·).

Null matrix: matrix where all the entries are 0.

$$0 \qquad \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \qquad \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Poperties: $A + O = O + A = A$ (both A and O here have same dimension),
$A + (-A) = O = (-A) + A$

Identity matrix: This is a matrix that has 1's in the lead diagonal and 0's everywhere else. (must be square)

EXAMPLE: $I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. $I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Properties: $AI_m = A$ (A is a $k \times m$ matrix), $I_nA = A$ (A is a $n \times p$ matrix).

$k \times m$ $m \times m$

$\frac{1}{2} \times 2 = 1.$

Inverse matrix

An inverse matrix is a matrix A^{-1} that has the property $A^{-1}A = I_n = AA^{-1}$. (Note: A must be square.)

EXAMPLE: Calculate the inverse, A^{-1}, of $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$. 2×2

Step 1: Calculate the determinant of A ($\det(A), |A|$) for a 2×2 matix $\det(A) = ad - bc$.

Step 2: Swap elements a and d. Multiply elements b and c by (-1). $\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

Step 3 : Multiply the matrix in Step 2 by $\frac{1}{\det(A)}$.

Thus, $A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = \frac{1}{ad-bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$.

EXAMPLE: $A = \begin{pmatrix} 3 & 2 \\ -2 & 1 \end{pmatrix}$. Find A^{-1}

Step 1: $\det(A) = 3 \times 1 - (-2) \times 2 = 7.$

Step 2: swap 3 & 1, multiply (-1) to 2 & -2.

$$\begin{pmatrix} 1 & -2 \\ 2 & 3 \end{pmatrix}$$

Step 3: $A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} 1 & -2 \\ 2 & 3 \end{pmatrix} = \frac{1}{7} \begin{pmatrix} 1 & -2 \\ 2 & 3 \end{pmatrix} = \begin{pmatrix} \frac{1}{7} & -\frac{2}{7} \\ \frac{2}{7} & \frac{3}{7} \end{pmatrix}.$

Note: not all square matrices have an inverse.

singular matrix. $\det(A)=0$

EXAMPLE: $A = \begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix}$

step 1: $\det(A) = 1\times2 - 1\times2 = 0$.

In step 2. we need to calculate $\frac{1}{\det(A)} = \frac{1}{0}$ ✗.

Only matrices whose det is non-zero is invertable.

Properties of inverses:

Transpose

$(A^{-1})^{-1} = A$ $\quad (A^T)^T = A$

$(AB)^{-1} = B^{-1}A^{-1}$ $\quad (AB)^T = B^TA^T$

$(A^\top)^{-1} = (A^{-1})^\top$

Types of matrices:

- Upper triangle matrix (right triangle matrix) has 0's in all entries below the lead diagonal.

e.g. $\begin{pmatrix} 1 & 1 & 2 \\ 0 & 2 & 3 \\ 0 & 0 & 1 \end{pmatrix}$

- Lower triangle matrix (left triangle matrix) has 0's in all entries above the lead diagonal.

e.g. $\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 0 & 0 \\ 2 & 1 & 4 & 0 \\ 2 & 3 & 4 & 5 \end{pmatrix}$

- Diagonal matrix only has entries in the lead diagonal, i.e., all other entries are 0's.

e.g. $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Simultaneous equations and matrices

EXAMPLE: Solve the following simultaneous equations using matrix methods:

$4x - 1y = 1$

$-2x + 3y = 12$

$$\underbrace{\begin{pmatrix} 4 & -1 \\ -2 & 3 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} x \\ y \end{pmatrix}}_{\underline{x}} = \underbrace{\begin{pmatrix} 1 \\ 12 \end{pmatrix}}_{\underline{b}}.$$

$$A \cdot \underline{x} = \underline{b}$$

$$\Rightarrow A^{-1} A \underline{x} = A^{-1} \underline{b}.$$

$$\Rightarrow \underline{x} = A^{-1} \underline{b}$$

$$\Rightarrow \underline{x} = A^{-1} \underline{b}$$

$$\Rightarrow \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 4 & -1 \\ -2 & 3 \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 12 \end{pmatrix}$$

Step 1: $\det(A) = 4 \times 3 - (-1) \times (-2) = 12 - 2 = 10.$

Step 2: $\begin{pmatrix} 3 & 1 \\ 2 & 4 \end{pmatrix}$

Step 3: $A^{-1} = \frac{1}{10} \begin{pmatrix} 3 & 1 \\ 2 & 4 \end{pmatrix}$

$$\Rightarrow \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 4 & -1 \\ -2 & 3 \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 12 \end{pmatrix} = \frac{1}{10} \begin{pmatrix} 3 & 1 \\ 2 & 4 \end{pmatrix} \begin{pmatrix} 1 \\ 12 \end{pmatrix} = \frac{1}{10} \begin{pmatrix} 3 \times 1 + 1 \times 12 \\ 2 \times 1 + 4 \times 12 \end{pmatrix}$$

$$= \frac{1}{10} \begin{pmatrix} 3 + 12 \\ 2 + 4 \times 12 \end{pmatrix} = \begin{pmatrix} \frac{15}{10} \\ \frac{50}{10} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{3}{2} \\ 5 \end{pmatrix}$$

i.e. $x = \frac{3}{2}$ $\quad y = 5.$