LECTURE-5

<u>Application to chemistry</u> : Balancing chemical equations assuming the following rule:

- <u>Conservation of mass</u>: No atoms are produced or destroyed in a chemical reaction.

<u>Example</u>: Consider the oxidation of ammonia to form nitric oxide and water, given by the chemical equation

$$(x_1)NH_3 + (x_2)O_2 \longrightarrow (x_3)NO + (x_4)H_2O.$$

Find the smallest positive integer values of x_1, x_2, x_3, x_4 such that the equation balances.

<u>Solution</u>: We equate the total number of each type of atoms on the two sides of the chemical equation:

atom N : $x_1 = x_3$

atom H : $3x_1 = 2x_4$

atom O : $2x_2 = x_3 + x_4$

These give rise to the following linear system :

$$\begin{aligned} x_1 \quad\quad - x_3 \quad\quad &= 0 \\ 3x_1 \quad\quad\quad\quad - 2x_4 &= 0 \\ 2x_2 - x_3 - x_4 &= 0 \end{aligned}$$

in the four variables with augmented matrix :

$$\left(\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 3 & 0 & 0 & -2 & 0 \\ 0 & 2 & -1 & -1 & 0 \end{array}\right)$$

which can be row-reduced to (check:)

$$\left(\begin{array}{cccc:c} 1 & 0 & -1 & 0 & 0 \\ 0 & 2 & -1 & -1 & 0 \\ 0 & 0 & 3 & -2 & 0 \end{array}\right)$$

leading to the general solution

$$(x_1, x_2, x_3, x_4) = t\left(\frac{2}{3}, \frac{5}{6}, \frac{2}{3}, 1\right)$$

if we assign the free variable $x_4 = t$.

the choice $t = 6$ gives the smallest positive integer solution:

$$(x_1, x_2, x_3, x_4) = (4, 5, 4, 6)$$

leading to the balanced equation:

$$4NH_3 + 5O_2 \longrightarrow 4NO + 6H_2O.$$

Review of matrix multiplication:

- $$\begin{bmatrix} a & b & c \\ * & * & * \\ * & * & * \end{bmatrix} \begin{bmatrix} d & * & * \\ e & * & * \\ f & * & * \end{bmatrix} = \begin{bmatrix} ad+be+cf & * & * \\ * & * & * \\ * & * & * \end{bmatrix}$$

2x2 example:

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 4 & 3 \end{bmatrix} = \begin{bmatrix} 1\cdot2 + 2\cdot4 & 1\cdot1+2\cdot3 \\ 2\cdot3+4\cdot4 & 3\cdot1+4\cdot3 \end{bmatrix}$$

$$= \begin{bmatrix} 10 & 7 \\ 22 & 15 \end{bmatrix}$$

- Rectangular matrices: Because rows of the first matrix are multiplied by the columns of the second matrix, observe that when multiplying AB, the no. of columns of A has to equal the no. of rows of B.

eg. $\begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 2 & 3 \\ 1 & -1 \end{bmatrix}$ → valid for multiplication

$\begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 2 & 3 \end{bmatrix}$ → not valid.

In general: $$A_{m \times n} \, B_{n \times p} = (AB)_{m \times p}$$

Recall:
Matrix multiplication is <u>NOT</u> commutative,
so $AB = BA$ need not be true.

Back to solving linear systems:

Recall: When trying to solve the linear eqn $ax = b$, we multiplied by a^{-1} on both sides, to get
$$x = a^{-1} b.$$

It would be convenient if we could carry this idea to matrices:

We can easily write a linear system in a single equation using the notation of matrices and vectors:

e.g.

$$\begin{aligned} x_1 + 2x_2 + 3x_3 &= -1 \\ 5x_1 + 11x_2 + 2x_3 &= 5 \\ x_2 - x_3 &= 10 \end{aligned}$$

can be expressed as:

$$\underbrace{\begin{bmatrix} 1 & 2 & 3 \\ 5 & 11 & 2 \\ 0 & 1 & -1 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}}_{\bar{x}} = \underbrace{\begin{bmatrix} -1 \\ 5 \\ 10 \end{bmatrix}}_{\bar{b}}$$

so $A\bar{x} = \bar{b}$, and in general:

$$\begin{aligned} a_{11}x_1 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + \cdots + a_{2n}x_n &= b_2 \\ &\vdots \\ a_{m1}x_1 + \cdots + a_{mn}x_n &= b_m \end{aligned} \quad \leftrightsquigarrow \quad \underbrace{A}_{m\times n}\ \underbrace{\bar{x}}_{n\times 1} = \underbrace{\bar{b}}_{m\times 1}.$$

We would like to understand: when can we just say $\bar{x} = A^{-1}\bar{b}$?

To do this, we need to define what is A^{-1}.
Inverse of a matrix using elementary row operations:

<u>Defn</u>: An $n \times n$ matrix is said to be invertible if there exists an $n \times n$ matrix B such that $AB = BA = I_n$.
(I_n: the $n \times n$ identity matrix)
In this case, we say that B is the inverse of A and write $B = A^{-1}$.

<u>Proposition</u>: Suppose A is an $n \times n$ invertible matrix. Then the inverse A^{-1} is unique.

<u>Proof</u>: We are given that A^{-1} exists. So, there is a matrix A^{-1} satisfying $AA^{-1} = A^{-1}A = I$.
Suppose B is any matrix satisfying $AB = BA = I$, we claim that $B = A^{-1}$, this would show that

the inverse matrix is unique.

Proof of claim:

$$A^{-1} = A^{-1}I = A^{-1}(AB) = (A^{-1}A)B = IB = B$$

because we know B satisfies $AB = I$

using associativity of matrix multiplication

Hence the inverse A^{-1} is unique.

Exercise: Suppose that A and B are invertible $n \times n$ matrices. Show that $(AB)^{-1} = B^{-1}A^{-1}$.

Now, we proceed to find the inverse of a matrix using elementary row operations.

Consider the following examples.

Let $A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$, $I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$.

(i) Let us interchange rows 1 and 2 of A, and do the same for I_3:

$$\begin{bmatrix} a_{21} & a_{22} & a_{23} \\ a_{11} & a_{12} & a_{13} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, \quad \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Observe that

$$\begin{bmatrix} a_{21} & a_{22} & a_{23} \\ a_{11} & a_{12} & a_{13} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

(ii) Let us interchange rows 2 and 3 of A and I_3. We obtain respectively:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{31} & a_{32} & a_{33} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} \text{ and } \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Observe that

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{31} & a_{32} & a_{33} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

(iii) Let us perform:

$$R_1 \mapsto R_1 - 2R_3$$

to both A and I_3. We get

$$\begin{bmatrix} a_{11}-2a_{31} & a_{12}-2a_{32} & a_{13}-2a_{33} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \quad \text{and}$$

$$\begin{bmatrix} 1 & 0 & -2 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Observe that

$$\begin{bmatrix} a_{11}-2a_{31} & a_{12}-2a_{32} & a_{13}-2a_{33} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & -2 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}.$$

(iv) Let us perform $R_2 \mapsto 5R_2$ to A and I_3:

We get:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 5a_{21} & 5a_{22} & 5a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

and observe that

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 5a_{21} & 5a_{22} & 5a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

What does this pattern above indicate?

Defn: An **elementary $n \times n$ matrix** is an $n \times n$ matrix obtained by performing an elementary row operation on I_n.

We have the following result:

Theorem: Suppose A is an $n \times n$ matrix and suppose that B is obtained from A by an elementary row operation. Suppose E is an elementary matrix obtained from I_n by the same elementary row operation. Then $B = EA$.

(proof omitted).