

Mathematics for Chemistry  
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Module – 03  
Lecture – 03  
Matrices, Matrix Operations and Determinants

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The image shows a whiteboard with handwritten notes on matrices. At the top center, the title "Matrices" is written. To the left is the NPTEL logo, and to the right is the IIT Kanpur logo. The notes include a 3x4 matrix:  $\begin{bmatrix} 1 & 3 & 4 & 1 \\ 2 & 2 & 1 & 3 \\ 0 & 2 & -1 & 7 \end{bmatrix}$ . Next to it, it says "→ Matrix" and "↓ Arrangement of scalars into rows and columns". Below this, it defines a square matrix as one where the number of rows equals the number of columns. The notation for a matrix  $A$  of size  $n \times m$  is shown as  $A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nm} \end{bmatrix}$ . Arrows point from the  $n$  and  $m$  in  $n \times m$  to "rows" and "columns" respectively. At the bottom, it explains that  $a_{ij}$  is the element in the  $i$ th row and  $j$ th column, and that a square matrix has  $m = n \Rightarrow A_{nn}$ .

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The image shows a whiteboard with handwritten notes in red ink. At the top left, there is a logo for NPTEL. The main content includes a 3x4 matrix:  $\begin{bmatrix} 1 & 3 & 4 & 1 \\ 2 & 2 & 1 & 3 \\ 0 & 2 & -1 & 7 \end{bmatrix}$ . To the right of this matrix, it says "Matrix" with a downward arrow, followed by "Arrangement of scalars into rows and columns" and "No of rows = No of columns". Below this, it defines a "Square matrix" as having "No of rows = No of columns". The notation for a matrix  $A$  is shown as  $A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nm} \end{bmatrix}$ . To the right of this notation, it says "n x m matrix" with arrows pointing to the number of rows and columns. At the bottom, it explains that  $a_{ij}$  is the element belonging to the  $i$ th row and  $j$ th column, and that a "SQUARE Matrix has  $m=n \Rightarrow A_{nn}$ ".

Today, we will start the discussion on matrices, matrix operations and determinants. So, let us get to matrices. So, what are matrices? So, visually we think of matrices as an arrangement of scalars. So, what we think of is that if you want the matrix, we represent it as some arrangement of scalars. So, for example, you could have you could have a matrix like 1, 3, 4, 1, 2, 2, 1, 3, 0, 2 minus 1, 7. So, this is an arrangement of scalars and this is referred to as a matrix. So, we can say that matrix is an arrangement of scalars into rows and columns.

So, a matrix has to be in general a rectangular object. So, you can also have what are called as square matrices. So, a square matrix implies number of rows equal to number of columns. So, now the notation we will use for a matrix, so notation for matrices if  $A$  denotes the matrix,  $A$  is a matrix, it is denoted by and rectangular array. And I will just start with it in general and then I will just explain to you what we are talking about. So, the elements of  $A$  are denoted as a little  $a_{11}$ ,  $a_{12}$ ,  $a_{13}$  up to a  $a_{1m}$ ; the second row you start with  $a_{21}$ ,  $a_{22}$ ,  $a_{23}$ , up to a  $a_{2m}$ , and you go all the way to the  $a_{n1}$ ,  $a_{n2}$ ,  $a_{n3}$ , all the way up to a  $a_{nm}$ . So, this matrix has  $n$  rows and  $m$  columns. So, we say this is an  $n$  by  $m$  matrix. So, this has  $n$  rows and  $n$  columns. And this notation is very useful where we just denote the various elements. So,  $a_{ij}$  is the element belonging to the  $i$ th row and  $j$ th column.

So, we will be following this notation throughout we will use capital letters to denote matrices, and small letters with the subscripts to denote the appropriate elements of matrices. Needless to say for a square matrix has m equal to n, so number of rows equal to number of columns. So, for a square matrix, so you typically have you denoted by A n n. So, it is an n by n square matrix. So, this is the basic of matrix. Now, when you can ask where is this useful and what are the properties of matrices?

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**Matrix Operations**  
**Addition and Multiplication**

NPTEL A (matrix) and B (matrix) can be added only if they have same no of rows & columns

$$A_{m \times n} + B_{m \times n} = C_{m \times n}$$

$$a_{ij} + b_{ij} = c_{ij} \quad \text{Rule for matrix addition}$$

$$A_{m \times k} B_{k \times n} = C_{m \times n}$$

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

Diagram illustrating matrix multiplication: A matrix of size m by k is multiplied by a matrix of size k by n to result in a matrix of size m by n. The diagram shows the dot product of a row from the first matrix and a column from the second matrix.

So, let us look at some basic properties of matrices So, I will just go through this very quickly because I am sure many of you are familiar with these. So, as far as addition and multiplication goes, so A, which is a matrix and B which is also a matrix, can be added only if they have same number of rows and columns. So, if you want to add 2 matrices, they should have the same dimensions, they should have the same number of rows and same number of columns. So, if you had A plus B, if it was C, then I can write that a i j plus b i j equal to c i j this is a rule for matrix addition.

So, what this means is that you have to add the element term by term that means, you have to add the i j th element of a to the i j th element of b to get the i j th element of c. So, if A is an m by n matrix and B should also be an m by n matrix and C also is an m by n matrix. What about multiplication? So, in multiplication, you can multiply an m by k matrix with a k by n matrix to get an m by n matrix. So, what I want to say is that you can multiply 2 matrices only if the number of columns of the first matrix is equal to the

number of rows of the second matrix. And the rule for matrix multiplication is that suppose I want to calculate  $c_{ij}$  the  $ij$ th element of  $C$ , then what I have to do is to sum over some other index, I will just call it  $l$  a  $l$  b  $l$  j. So, I sum over all  $l$  and  $l$  should go from 1 to  $k$ .

So, again I am not doing this in all detail because I am sure many of you are familiar. So, if you have a matrix that looks like this, and you have another matrix that looks like this, where the number of rows here is equal to the number of columns here. Then when you multiply these you will get a matrix that has this many rows and this many columns. So, you will get a matrix that has this many rows and this many columns. So, if this is  $m$ , and this is  $k$ , this is  $k$ , and this is  $n$ , then this is  $m$  and this  $n$   $m$  by  $n$  matrix. And the way you get it is you take the elements of the row and you multiply them by the elements of the column.

Suppose, I want to find the first element of this of this matrix, then I have taken the element of the first row and the first column of  $n$  and multiply first I multiply these 2 then I multiply these 2. Then I multiply these 2 and I go on and on, then I multiply these 2 and then I go on and on till I reach the end. So, you have to multiply them term by term. So, this element multiplied this element this element multiplies this element this element multiplies this element and so on all the way up to the end; and when you do that you when you add all of them up you will get this particular element.

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**Matrix Operations**  
**Transpose and Trace**

Restrict to Square Matrices

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \quad \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}$$

$A \quad A^T$

$a_{ij} \leftrightarrow a_{ji}$   
 $A \leftrightarrow A^T$

Trace = Sum of  $n$  Diagonal Elements  

$$\text{Tr} [A] = \sum_{i=1}^n a_{ii}$$

So, that is so much for addition and multiplication of matrices, there are a couple of other operations that you can do one is called a transpose of a matrix. So, we will; again will restrict discussion to square matrices that is  $m$  equal to  $n$ . So, suppose you have a matrix  $A$ , which is a square matrix  $A$  and  $A$  transpose is, so this is  $a_{11}$ ,  $a_{12}$ , up to  $a_{1n}$ ,  $a_{21}$ ,  $a_{22}$ , up to  $a_{2n}$ ,  $a_{n1}$ ,  $a_{n2}$ , up to  $a_{nn}$ . Then if this is  $A$ ,  $A$  transpose is given by the matrix where the rows and columns are swapped. So, what you have is  $a_{11}$ ,  $a_{12}$ , up to  $a_{1n}$ ,  $a_{21}$ ,  $a_{22}$ , up to  $a_{2n}$ ,  $a_{n1}$ ,  $a_{n2}$ , up to  $a_{nn}$ , so that is  $A$  transpose. So, I can write  $a_{ij}$  is your element of  $A$  then the corresponding element of  $A$  transpose is  $a_{ji}$ . So,  $a_{ij}$  and  $a_{ji}$  are swapped in  $A$  and  $A$  transpose. So, when you go from  $A$  to  $A$  transpose, you are swapping the off diagonal elements the diagonal elements are not affected, because  $a_{ii}$  remains the same.

The next thing is called the trace. So, trace of a matrix again will restrict to square matrix. So, trace equal to sum of diagonal elements. So, trace of  $A$  is equal to sum over  $i$  equal to 1 to  $n$   $a_{ii}$ . So, this trace sometimes plays a role in various operations. So, these are some basic matrix operations.

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**Matrix Operations**  
**Determinants**

NPTEL Only for Square Matrices

$$\text{Det } A = a_{11}(\text{cof } a_{11}) + a_{12}(\text{cof } a_{12}) + \dots + a_{1n}(\text{cof } a_{1n})$$

$$= \sum a_{1i} \text{Cof}(a_{1i})$$

$$A_{3 \times 3} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \quad \text{Det } A = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}(a_{22}a_{33} - a_{23}a_{32}) - a_{12}(a_{23}a_{31} - a_{21}a_{33}) + a_{13}(a_{21}a_{32} - a_{22}a_{31})$$

$$\text{Cof } a_{11} = a_{22}a_{33} - a_{32}a_{23}$$

$$= \text{Det} \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix}$$

Cofactor is the determinant of the matrix with one row and one column removed

Each term in determinant has a product involving exactly 1 element from each row and each column.

There are some other useful operations or objects that are defined in relation to matrix and this is a determinant. So, suppose you have again only for square matrices, determinants are only defined for square matrices. So, if you have a matrix  $A$  which is an  $n$  by  $n$  matrix then you can write determinant of  $A$ , you can write it as in the following

way. So, what you will do is you will write it as a  $1 \times 1$  times write this as what is called a cofactor of a  $1 \times 1$  plus a  $1 \times 2$  times cofactor of a  $1 \times 2$  plus dot, dot, dot up to a  $1 \times n$  times cofactor of a  $1 \times n$ .

I will just explain what this is to motivate the determinant we kind. So,  $i$  can  $i$  can write this in general as a sum over  $i$  a  $1 \times i$  times cofactor of a  $1 \times i$ . So, I will come to what the cofactor is, but for us to initiate the discussion suppose you have a  $3 \times 3$  matrix suppose you have a  $3 \times 3$ . So, this is denoted by a  $1 \times 1$ , a  $1 \times 2$ , a  $1 \times 3$ , a  $2 \times 1$ , a  $2 \times 2$ , a  $2 \times 3$ , a  $3 \times 1$ , a  $3 \times 2$ , a  $3 \times 3$ . So, this is my matrix  $A$  then determinant of  $A$  is denoted by the same matrix with straight lines. So, instead of the square brackets you have straight lines  $a_{12}$ ,  $a_{13}$ ,  $a_{21}$ ,  $a_{22}$ ,  $a_{23}$ ,  $a_{31}$ ,  $a_{32}$ ,  $a_{33}$ . And this is equal to I will write it in three lines here. So, it is a  $1 \times 1$  times a  $2 \times 2$  into a  $3 \times 3$  minus a  $2 \times 3$  into a  $3 \times 2$  plus a  $1 \times 2$  into a  $2 \times 3$  into a  $3 \times 1$  minus a  $2 \times 1$  into a  $3 \times 3$  plus a  $1 \times 3$  into a  $2 \times 1$  a  $3 \times 2$  minus a  $3 \times 1$  a  $2 \times 2$ . So, it is a sum of three terms, just as you can see from this expression that it is a sum of three terms.

So, how did we calculate the determinant we multiplied this a  $1 \times 1$  by what is called the cofactor which is nothing but this determinant. Then we multiplied a  $2 \times 2$  sorry, show it with different color with this. So, you remove this row and this column. So, if  $i$  imagine that I take out this row and this column then I get this determinant which starts with a  $a_{23}$ ,  $a_{33}$ ,  $a_{21}$ ,  $a_{31}$ . So, I just have the value of that determinant a  $2 \times 3$  times a  $3 \times 1$  minus a  $2 \times 1$  times a  $3 \times 3$ . Similarly for a  $3 \times 1$  what I do is I remove this row and this column and  $i$  multiplied by this factor, so that is the basic idea of it determinants that you write it in terms of these cofactors.

So, just to remind, so cofactor of a  $1 \times 1$  is equal to a  $2 \times 2$  times a  $3 \times 3$  minus a  $3 \times 2$  times a  $2 \times 3$ , this is nothing but determinant of the matrix formed by removing this row and this column. So, a  $2 \times 2$ , a  $2 \times 3$ , a  $3 \times 2$ , a  $3 \times 3$ , so, this is the basic idea. And you can do this for larger matrices also but you will have to calculate more and more determinant. So, this cofactor is nothing but the determinant of a smaller matrix, cofactor is the determinant of the matrix with one row and one column removed.

So, now that we have the idea of determinant, we can go ahead to the next operation. I will also mention one more thing that if you look at any term in the determinant, it will have a product of 3 of the elements of the matrix. So, for example, this term a  $1 \times 1$  times a  $2 \times 2$  times a  $2 \times 3$  is a product of a  $1 \times 1$  times a  $2 \times 2$  times a  $3 \times 3$ . The next term which is a  $1 \times 1$

times a 2 3 times a 3 2 is a product of this times this times this. So, each term in the determinant contains exactly one element from each row and each column. So, there is a exactly one element from each row in each column, you can never have a product that involves 2 elements from the same row or 2 elements from the same column. Every product has one element from each row and one element from each column. I will just make a note of this each term in determinant has a product involving exactly one element from each row and each column. And this is again a very, very important fact to note that you never have 2 elements from the same row multiplied in a determinant you know determinant expression.

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**Matrix Operations**  
**Inverse**

Square Matrices only

Identity matrix  $I_{n \times n} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix}$

$A I_{n \times n} = A_{n \times n}$

Suppose  $AB = I$ , then  $B$  is called inverse of  $A$  and  $B = A^{-1}$

$AA^{-1} = I = A^{-1}A$

Inverse of matrix  $A$

The next operation for matrix is so this has to do with inverse and in order to define the inverse again this is only for square matrices. So, in order to define the inverse we define something called an identity matrix I. If you have an n by n matrix, so this is the diagonal elements are 1, and all the off diagonal elements are 0. So, all these all the off diagonal elements are 0, all the diagonal elements are 1, so that is what is called an identity matrix. And identity matrix has the property that any matrix multiplied by the identity matrix gives you A, gives you the same matrix that means, and again let us restrict to square matrices.

So, let us take an n by n matrix and you take an n by n matrix you get A, it is n by n. So, an identity matrix is like the unit in multiplication it is like 1. So, any scalar multiplied

by 1 gives you the same scalar. So, any matrix multiplied by identities gives to the same matrix, so it is like your 1. So, now you can ask suppose A times B equal to identity then B is called inverse of A, and we can write B equal to A inverse. So, in other words A times A inverse is equal to identity which is also equal to A inverse times A again it is not have to show this but basically A times A inverse is identity and. So, now, we have defined the inverse of a matrix, this is inverse of matrix A. So, inverse of a square matrix is also a square matrix and again the matrix inverses of something that we end up using a lot.

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**Matrix Operations**  
**Row and Column Operations**

NPTEL

Column operations can be similarly defined

Row and Column operations leave determinant unchanged

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Row operation:  $R_2 = R_2 + cR_1$

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \xrightarrow{R_2 + cR_1} \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} + ca_{11} & a_{22} + ca_{12} & \dots & a_{2n} + ca_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}$$

Column operation:  $C_2 = C_2 + dC_1$

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \xrightarrow{C_2 + dC_1} \begin{bmatrix} a_{11} & a_{12} + da_{11} & \dots & a_{1n} \\ a_{21} & a_{22} + da_{21} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} + da_{n1} & \dots & a_{nn} \end{bmatrix}$$

Matrix operation that I want to talk about is that of row and column operations. So, suppose you have a matrix A, I will just take a simple matrix A denoted by a 1 1, a 1 2 or usual make it should be a 1 n, a 2 1, a 2 2, a 2 n, a n 1, a n 2, a n n. And I can do this for square or rectangular matrices. Now, a row matrix, so a row operation is something like, so suppose you take R 2 plus c times R 1. So, what you mean by this is row 2 plus c times row 1, and then you call this as row 2 is equal to row 2 plus c times row 1. So, what you mean you will get a new matrix. What does that new matrix look like, it looks like the first row is unchanged to the second row you add c times the first row, and you have to do it element by element.

So, what you do is this element becomes a 2 1 plus c a 1 1. Similarly, this element becomes a 2 2 plus c a 1 2, and the last element becomes a 2 n plus c a 1 n, and all the



other elements remain unchanged. So, only row 2 is changed by this operation, this is called a row operation. You can do you can multiply any constant you can subtract and you can add 2 different rows and so on. So, this is called a row operation, where you add one row to another row, add or you take linear combination of rows.

You can also have column operations. So, column operations can be similarly defined so for example, if you have the same matrix  $A$ , which is an  $n$  by  $n$  matrix. And you do a column operation, where let say we do  $C_2$  equal to  $C_2$  plus  $d$  times  $C_1$ . So, what does that mean, that means, you do not do anything to column 1  $a_{11}$ ,  $a_{21}$ , up to  $a_{n1}$ ; but to column 2, you add  $d$  times column one. So, what you will get is  $a_{12}$  plus  $d a_{11}$ ,  $a_{22}$  plus  $a_{21}$  and all the way up to  $a_{n2}$  plus  $d a_{n1}$ , and then all the other elements unchanged all the other columns are unchanged. So, what you did by this is by this row and column operations, you get new matrices. And there are some interesting properties of these row and column operations. One of the things is that is that when you do these row and column operations the determinant is unchanged. So, row and column operations leave determinant unchanged. You can show that row and column operations leave the determinants unchanged. We will discuss some properties of determinant a little later, but we will just keep in mind right now that when you do row and column operations, then that determinant of the matrix is not changed.

Thank you.