Advanced Mathematical Methods for Chemistry
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Module - 02
Lecture - 04
Determinants, Matrix Inverse

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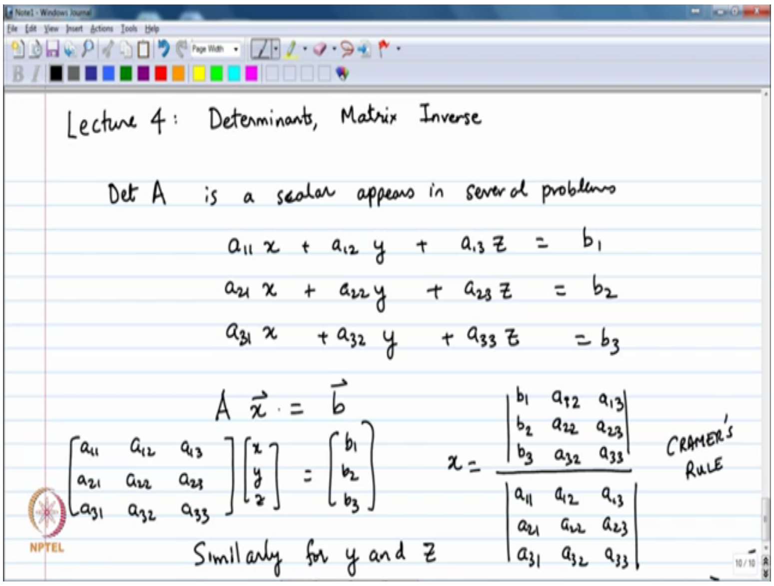

So, in the next lecture we will be talking about determinants and inverses of matrices. So, what is a determinant of a matrix? A determinant of matrix is a scalar that appears and this determinant appears in lot of problems in several problems. For example, suppose you add a 11 x plus a 12 y plus a 13 z equal to b 1, a 21 x plus a 22 y plus a 23 z equal to b 2, a 31 x plus a 32 y plus a 33 z equal to b 3. So, suppose you had a system of equations, so we can write this as a times x equal to b where x is basically this is x y z, b as b 1 b 2 b 3 and a is this matrix. So, this is a matrix and a x equal to b. So, you can write these equations in this form.

And now you can to solve this your goal is to solve this. So, suppose you know a and b you want to solve this to for x, and you can solve this and you can show that when you solve this you will get you can write x as equal to the following I will just write it, I will just write that is the answer this is. So, you write a determinant of a 11 a 12 a 13, a 21 a 22 a 23, a 31 a 32 a 33. So, this is just the determinant of a.

And what you do in the, so this appears in the denominator in the numerator what you have is you have something like the determinant of a, but you replace the first column by b. So, what you do is you replace the first column with the vector b 1 b 2 b 3 and you take the determinant of that. Similarly if you want to calculate for y then you replace the second column of a with b 1 b 2 b 3. So, this is called, this is called as Cramer's rule. So, you can do similarly for y and z. So, I will just I will just write you can do similarly for y and z.

So, basically you can solve this set of equations in and determine x y and z and you can do this for an arbitrary sized matrix you can do for arbitrary number of equations. So, if you have more equations you will have bigger matrices. So, this is one place where determinants appear most naturally and we also saw that determinants also appear in determinants are involved in calculating eigenvalues of a matrix.

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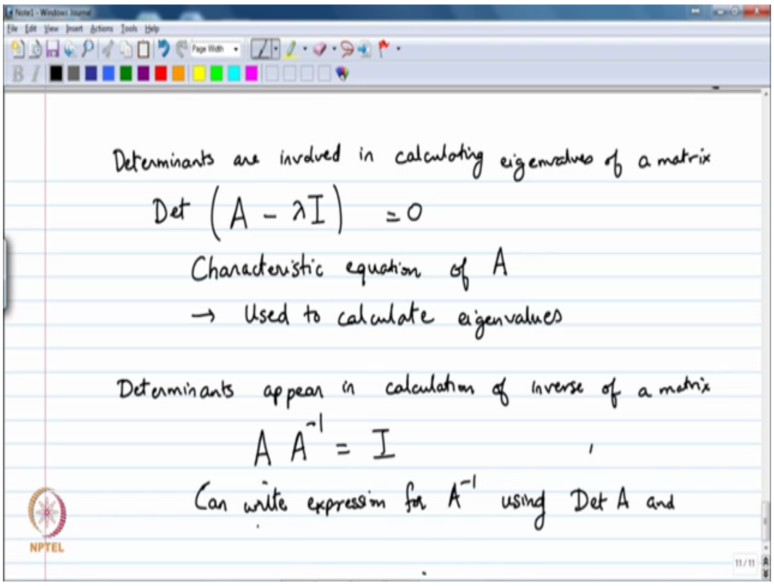

And we already saw that that suppose you want to calculate an eigenvalue of a matrix a then you just you just take this matrix A minus lambda I and you set its determinant equal to 0. So, this is referred to as the characteristic equation of A. So, it is a characteristic it is called the characteristic equation because the eigenvalues are often called the eigenvalues refers to as the characteristic of A, and this is used to calculate used to calculate eigenvalues. And we know that this leads to a polynomial equation in lambda.

So, determinants are very naturally involved in calculating eigenvalues of a matrix another place where the determinants are involved is in calculating the inverse of A matrix. So, in calculation of inverse of a matrix, suppose you had a square matrix A then we know that A times A inverse equal to identity and it turns out that you can you can express you can express and write expression for A inverse using a determinant of A and determinants of water of various matrices involving various matrices of which are obtained from A. So, we can use various matrices that are obtained from A and those determinants are also involved in calculating the inverse of A.

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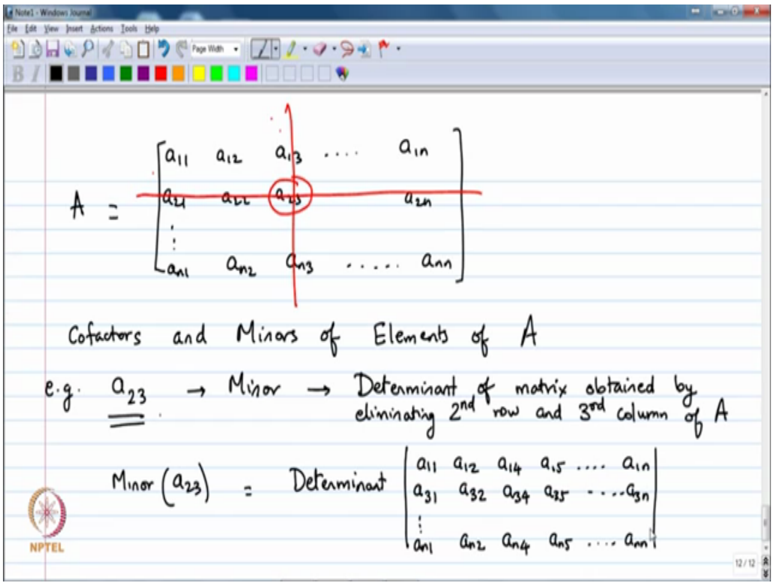

So, this is the next use of a determinants and just to illustrate suppose you have a matrix A which has these terms a 11 a 12 a 13 up to a 1n, a 21 a 22 up to a 2 n and a n1 a n2 a n3 up to a nn. So, suppose you have this matrix A. Now you can determine, you can you can you can determine what is the cofactor. So, the cofactors and minors of elements of A, for example, if you take a ij or let me let me take a specific example for example, if you take a 23. So, this is an example consider a 23.

Now, if you want to find the cofactor of a 23 or the minor of a 23. So, what you do? So, first let us say the minor of a 23. So, minor nothing, but determinant of matrix obtained by eliminating, so what is done is you want to determine the cofactor of this element a 23. So, what you do is you make a matrix you look at this matrix. So, you look at this matrix where you have n minus 1 rows and n minus 1 columns. So, 1 fewer row and 1 fewer column and what you can say is that minor of a 23 is nothing, but determinant of this matrix a 11 a 12 then you eliminate the third column, so you have a 14 a 15 up to a 1n then you have a you eliminated the second row. So, you have a 31 a 32 a 34 a 35 up to a 3n all the way up to a n1 a n2 a n4 a n5 a nn. So, this is what is meant by the minor of a 23 and similarly the cofactor we have the minor determined of each element defined in this way.

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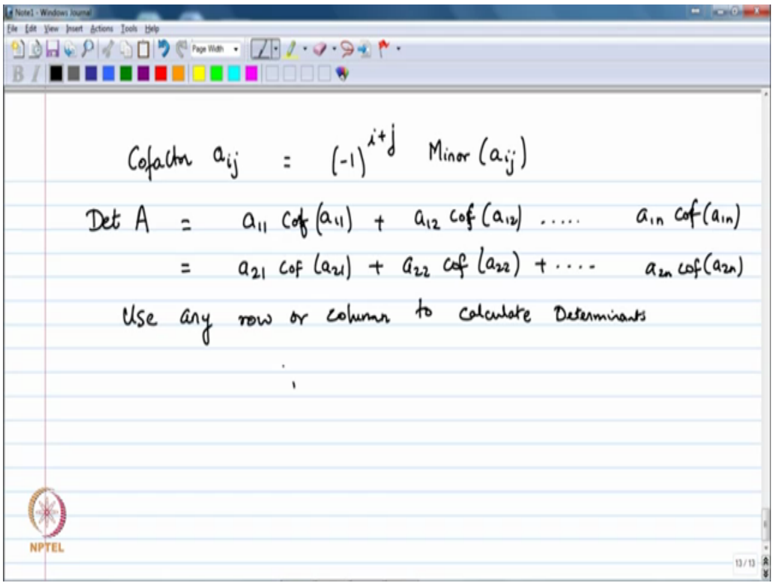

Now, there is something called a cofactor. So, cofactor of an element a ij a ij is the element of a this is nothing, but minus 1 raised to I plus j times minor of a ij. So, you just take a ij and multiplied by a plus or minus 1 depending on whether i plus j is odd or even. So, this is the cofactor of a and what this allows you to do is 2 things one is you can write you can show that determinant of a is equal to a 11 cofactor of, cofactor of a 11 plus a 12 times cofactor of a 12 and so on all the way up to a 1n times cofactor of a 1n. So, you can expand the determinant in terms of cofactors.

This is again you can easily verify this and I chose. So, can you can do this using any row or any column. So, you can also write this as a 21 cofactor of a 21 plus a 22 times cofactor of a 22 plus a 2n times cofactor of a 2n. So, we can use any row or column to calculate determinants. So, the minor of a is of any element of this a half of the matrix a is given in this way.

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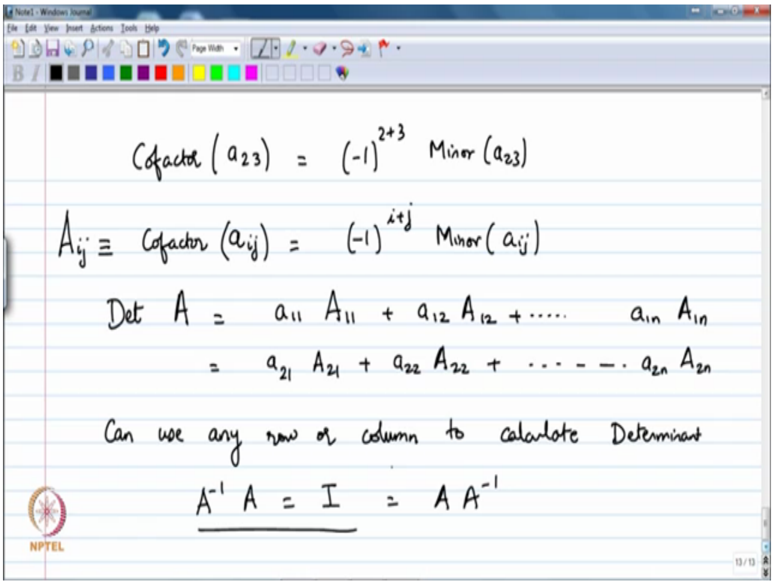

Similarly, we can there is something called a cofactor which is defined based on the minor. So, cofactor again this is cofactor of an element let us say if you have a 23 this is minus 1 raised to 2 plus 3 times minor of a 23. So, this is basically this is minus 1 times minor of a 23. In general cofactor of a ij, we will use the notation capital A ij this corresponds to the cofactor of a ij this is equal to minus 1 raised to i plus j times minor of a ij. So, the cofactor of an element is minus 1 raised to i plus j times minor of a ij and the cofactors are very useful because I can write a determinant of a as a 11 times cofactor of a 11 plus a 12 times cofactor of a 12 plus so on a 1n times cofactor of a 1n.

So, I just take the elements of the first row and I multiply them by their cofactors and add all of them and I will get the determinant of the a. I can similarly, I can use some other row I can use let us say a 21 times cofactor of a 21 plus a 22 times cofactor of a 22 plus all the way up to a 2n times cofactor of a 2n or I can use any column. So, we can use any row or column to calculate determinant.

So, these cofactors and minors are they play a role in calculation of determinants. They also play a role when you are calculating the inverse of a matrix. So, we already saw that that a inverse times a is the identity matrix and this is equal to a times a inverse. So, this is the definition of the inverse. Now suppose you know the elements of a, suppose your a is expressed in the usual way. Then you define a matrix of cofactors.

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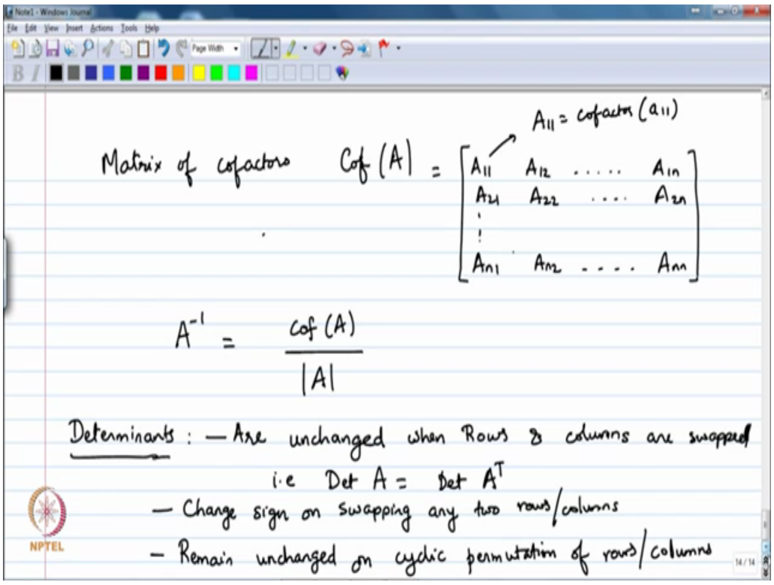

So, this I call it as I will just call it as cofactor of A of this matrix this is a matrix whose elements are nothing, but the cofactors of A. So, so this will be A 11 A 12 up to A 1n, and then A 21 A 22 notice it is capital A which is the cofactor A 2n A n1 A n2 up to A nn.

So, instead of putting the element you put the cofactor of that element instead of putting little a 11, I put capital A 11 which is the cofactor of this is A 11 equal to cofactor of a 11. So, this matrix of cofactors can be used to calculate the determinant. So, A inverse is equal to cofactor of A divided by determinant of A, this is the matrix of cofactors divided by the determinant of A which is nothing but the inverse of the matrix. So, you can calculate the matrix inverse and as I said cofactors this is the matrix of cofactors. So, so this is the matrix of cofactors you divide that by determinant which is a scalar. So, you will get a matrix and this is the expression for the inverse of a matrix.

We have seen how to calculate inverse of a matrix and what are the uses of determinants, now let me briefly mention a few properties of determinants that are of interest. So, determinants since these appear very often. So, some properties of determinants that are of interest is that they are unchanged when rows and columns are swapped, are swapped that is in other words determinant of A equal to determinant of A transpose of the transpose matrix. They change sign on swapping any 2 rows or columns. If you interchange any 2 rows or any 2 columns then the determinant will change sign it will become negative of that.

The other thing, other 2 important points are that they are they remain unchanged on cyclic permutation of rows or columns.

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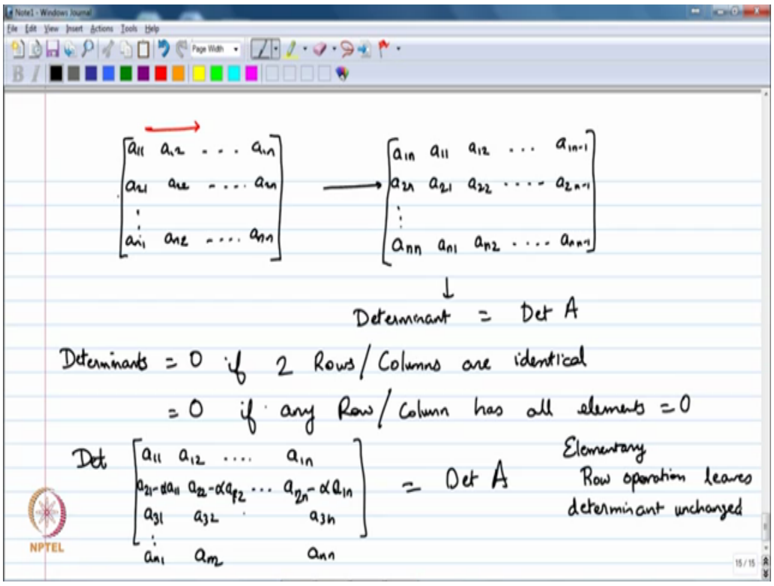

If I shift all the rows or columns to the right, for example, if I take this matrix and let us say this is a 11 a 12 up to a 1n, a 21 a 22 up to a 2 n and so on and I take this matrix and then I do, I sort of shift everything to the right by 1. So, what I do is I take I put a 11 here a 1n minus 1 and I take an and I put it here a n1 and I put or a 1n and I put it here. So, what I did is I shifted everything to the right by 1. So, you shift everything to the right by 1 and you do this for all the columns. So, this will be a 2n a 21 a 22 a 2n minus 1 a nn a n1 a n2. So, now that when you do the cyclic permutation of rows or columns then the determinant is unchanged. So, determinant of this matrix equal to determinant of a, so a determinant remains unchanged on cyclic permutation of rows you can do that for columns also.

The next probably, another very important use of determinants is that determinants determinant equal to 0 if 2 rows or columns are identical. So, if any 2 rows or any 2 columns are identical then the determinant is 0 of course, if any row or column, if any row or column has all elements equal to 0. So, if any row or column has all the elements equal to 0 then the determinant is unchanged is equal to 0.

So, what this implies is that determinant of let us say you consider you take you do something like this. So, you have a 11 a 12 up to a 1n then instead of a 21 you do something like a 21 minus alpha a 11 a 22 minus alpha a 12 a 2n minus alpha a 1n and you take and you leave again you leave the rest of them the same - a 31 a 32 up to a 3n, a n1 a n2 up to a nn and you take the determinant of this matrix. So, this is equal to the determinant of A.

Now, what did you do here? You took the second row and you subtracted alpha times the first row. So, you did you did a row operation what is called an elementary row operation row operation and you found that this leaves determinant unchanged. So, this is again a very very important idea that if you take, if you take a matrix you do an elementary row you can do an elementary column operation also you can do for any row or any column. If you do these operations then the determinant is unchanged. So, now, these are some of the important properties of determinants that make them very very useful in various applications.

So, I will conclude this lecture here and in the next class we will try to do some practice problems involving all these concepts.