Mathematics for Chemistry
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Lecture - 10

We have looked at the usefulness of the rank of a matrix and we have seen how the rank tells us, whether a set of equations is solvable or not and whether solutions exist and if they exist is there a unique solution or are there infinitely many solutions. So, clearly the rank of a matrix is a very useful quantity to have to know especially when we are dealing with very large number of equation, so often in many theoretical studies you be deal with matrixes of very large orders of the thousands, and we need to have an efficient way to calculate the rank of the matrix. So the rank is defined as the number of linearly independent rows or columns of the matrix.

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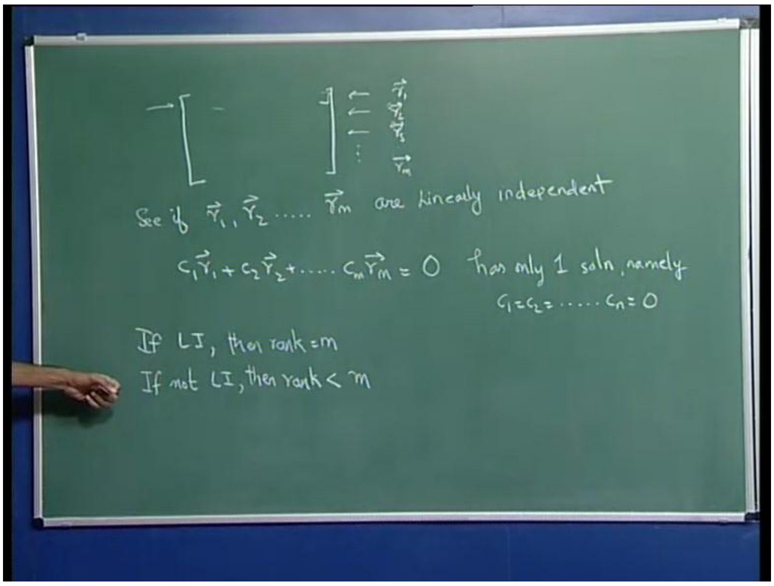

So, the obvious way to determine the rank would be that you consider if you think of a matrix, where the elements of the first row, we call them r 1 vector, you can think of them as r 1 vector, elements of the second row we think of r 2 vector, elements of the third row as r 3 vector and so on. So, the elements of the first row all these elements can be thought of as a vector and we can call that vector r 1. Similarly, the elements of the second row we call it vector r 2 and r 3 and so on.

Now, we are asked to determine the rank and we have to find out how many of these vectors are linearly independent. Now, so the first thing to do is to see if these see if all these vectors are linearly independent, so we have a total of let us say r m, so first we see if all the vectors are linearly independent. So, see if and let me remind you that these vectors are said to be linearly independent, if the Equation c 1, r 1 plus c 2, r 2,c m, r m equal to 0 has only 1 solution namely c 1 equal to c 2, equal to c n, equal to 0.

So, if this equation has only 1 solution and that is the trivial solution and no other solution, then these vectors r 1, r 2 up to r m are said to be linearly independent. So, we check for linear independence and if these vectors turn out to be linearly independent, if linearly independent then clearly the rank should be equal to m and if it is not linearly independent then the rank is less than m.

So, if not linearly independent then rank less than m so now we have to say what the value of this rank is some number between 1 and m but we do not what it is; so then what we do is we take various sub sets of m minus 1 vectors. So, you can take the first m minus 1 vectors and you can see whether, they are linearly independent and you keep repeating this process, if they are linearly independent then the rank is m minus 1, if they are not linearly independent then the rank is less than m minus 1.

So, you keep repeating till you reach a set of vectors, that are linearly independent and that is what you identify as a rank. So, we go almost through this iterative procedure we will first check, if rank is equal to m then if it not equal to m then it must be less than m. So, then you check if rank equal to m minus 1 and so on.

Now clearly, you can see that this procedure is quite compression and you know that you can check, whether the rank is 0 of a matrix but sorry, you can check if the rank is M. But, after that you have to take subsets of these vector and then try to look for smaller rank and clearly, this procedure will work for if you have a few vectors, but if you have a very large number of vectors this procedure is not very efficient and the procedure that is used is something called Gauss elimination.

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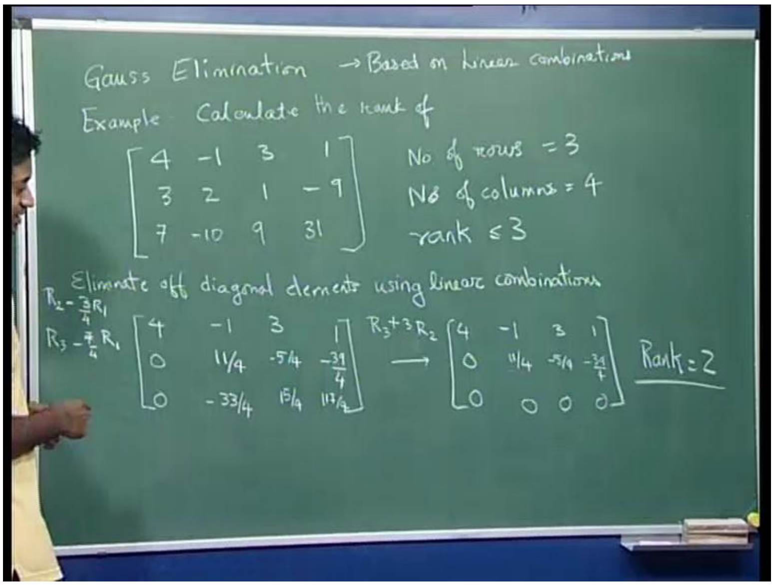

And this is based on the taking linear combinations of vectors and I would not go in to the detail of you know the formal procedure, what I will show is I will illustrate this through an example. Now suppose you have to calculate example, calculate the rank of in the matrix is given by 4 minus 1 3 1 3 2 1 minus 9 7 minus 10 9 31.

So you are asked to calculate the rank of this matrix, now you while it is worth mentioning now that though, I did this with rows, I could also do this with columns and you can choose to do it with which ever elements you like, if you want to do it with rows, you can do it with rows, if you want to do it with columns, you can do it with columns and the answer will be the same, so that is the important point. Now here the number of rows is 3 number of column is 4 so you say that number of rows equal to 3 number of columns equal to 4 and this clearly implies that rank has to be less than equal to 3.

So, it can either be 1, 2 or 3 and so let us work with the rows, now in Gauss elimination, if you are working with the rows the what you try to do is to try to eliminate the elements that are off diagonal, using linear combinations. So, in this case let us see how this works, so if you take this matrix and you take here you have a 3, you have a 4. So, if you want to eliminate this, you subtract 3 4 from this row, so we take the first.

So, we take the second row and subtract 3 4 of the first row, so if you do that the first row remains as it is you do not do anything to it, so if I subtract 3 4 of the first row, I will get rid of this element. Now, here if I subtract 3 4 so it is 2 minus 3 by first, so I will say I will call this as R 2 minus 3 by 4 R 1, so from the second row you subtract 3 4 of the first row and if, you do this you will get 2 plus 3 by 4 that is 11 by 4, this is 1 minus 3 by 4 that is 1 by 4, this is minus 9 minus 1 by 4, so it is minus 37 by 4, then for the third row we want to convert this to 0.

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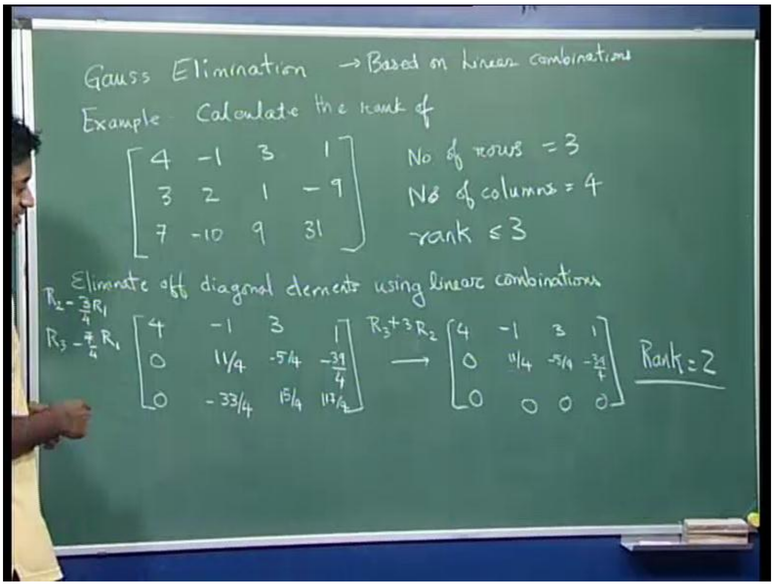

So, what we will do is R 3 minus 7 by 4 R 1 so from the third elements you subtract 7 4 of the first row and what you will get is 0 and if I subtract 7 4 here. So minus 10 minus 7 by 4 that is the minus 10 plus 7 by 4, so that is minus 40 plus 7 minus 33 by 4, 9 minus 7 by 4 into 3 let me make sure, I got this correct. So, in this case I had 2 plus 3 by 4 and you had 1 minus 3 into 3 9 by 4, sorry so that should this is not correct. So, this should read this is minus 37 by 4 so 1 minus 3 by 4 of 1.

So, 9 minus 3 by 4, so minus 9 is minus 36 by 4, so minus 39 by 4 then minus 1, sorry 1 minus 3 into 3 by 4, 3 into 3 is 9 by 4 is so 1 minus 9 by 4 is minus 5 by 4. Now in this case this minus 7 4 of this gives you 0 minus 10 minus 7 by 4 into minus 1, so that is minus 10 plus 7 by 4, so that is minus 33 by 4, 9 minus 3 into 7 21 by 4, that is 15 by 4. And similarly, 31 minus 7 by 4 and that is 34 minus 7 1 1 7 by 4, so in this way you have eliminated by choosing suitable linear combinations we have eliminated these 2 rows.

Now, next what we want to do is to take linear combinations and eliminated this element so in order to eliminate that what we will do is will operate by will we will carry out the operation R 3 minus, now if, I add 3 by 4 R 2, then I will eliminate this row so then I will eliminate this number. So, to in order to eliminate this I will do 33, so minus 33 by 4 plus 33 by 4, so I will get 0. And notice that this operation does not change this, so this plus 3 by 4 of this gives still gives me 0, so I have 4 minus 1 3 1 0 11 by 4, now this operation will not change the second row minus 5 by 4 minus 39 by 4 and when I do this.

So, the first row so the third row element was 0, I add 3 4 of 0, I still get 0, if I take this add 3 times sorry, not 3 4 if, I add 3 times this element then I will get minus 33 plus 33 by 4, so that is 0 here if, I add 3 times I will get again 0. So, 15 by 4 3 times 5 by 4 is 15 by 4, so 15 by 4 minus 15 by 4, I get 0 and again if, 3 times this 39 times 3 is exactly 100 and 70, so again I will get 0. So, now by doing various eliminations, we have managed to get 1 full row to be 0 and 3 are 2 non zero rows and it is not hard to show, that you can never convert this row completely to 0 so if you try to do anything, if you try to convert this element to 0, you will make this element non zero.

So, there is no way of converting all these elements to 0 and so we have 2 so after linear combinations we are left with 2 rows so these 2 rows are linearly independent or rank equal to 2. So, the procedure for finding rank is to keep doing Gaussian eliminations and find out how many non zero rows survive, at the end of this process of Gaussian elimination and the process of Gaussian elimination is to try to get 0’s on in as many rows as possible starting. So, you start from the lower triangular apart and try to get as many 0’s as possible and you can easily show that this will lead to a rank of 2, so because you are left with 2 independent rows.

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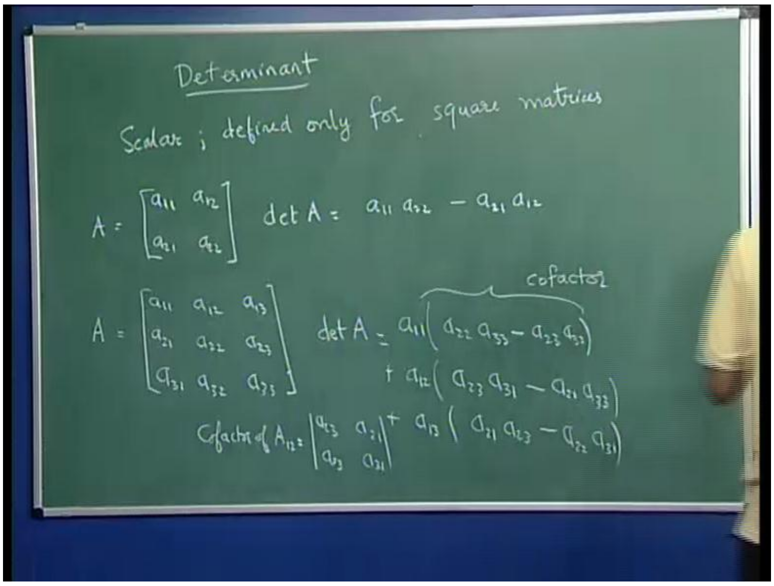

The next concept that we do involving matrices is a concept of a of the determinant of a matrix so the determinant of a matrix is a scalar. So, the scalar quantity and it is defined only for square matrices so the determinant is only defined for square matrixes and it is a scalar and this is a scalar, that appears quite often when we are dealing with various system of equations and therefore, we will go and we will try to give the formal definition of this. Now if you had a 2 by 2 matrix then the if, a is a 2 by 2 matrix, then determinant a is just a 11 a 22 minus a 21 a 12.

So, the determinant is defined as, the as a product of these 2 elements minus the product of these 2 elements and you might also be familiar that, if you had a 3 by 3 matrix. Then the determinant of a is given by a 11 times determinant of this matrix, which is a22 a 33 minus a 23 a 32. So, we took these times the determinant of this matrix then you take this times the determinant of this matrix. So, that is plus a 12 times a 23 a 31 minus a 2123312133 then plus a 13 a 13 times the determinant of this matrix that is a 21 a 23 minus a 22 a 31.

So, the point is once you have the determinant of a smaller matrix defined you can calculate the determinant of larger matrices and you can extend this procedure further. So notice what we did, we started with a row and we took the first element and multiplied by the determinant of the matrix, that is obtained by removing this row and this column. Then you took the second element and you removed this row and this column and you get a matrix that is a 32 a 33 a 21 a 31 and you take the determinant of that then you go to a 31 remove these 2 rows. This row and this column and you get this matrix.

So, you take the determinant of that so this is the general procedure and you can extend this to once you have defined, it for small matrices you can define for larger matrices now the definition involves will always involve this quantity which is the determinant of the matrix obtained by removing the row and the columns. It will always involve this quantity so we will give it a name. So, if we preserve the order of the matrix then this element is called the cofactor so this element is called the cofactor and notice that in the cofactor you preserve the order. So, if you are looking at the cofactor of a 12 at the cofactor of a 12 is equal to determinant of a 23 a 33 a 21 a 31 and you can define the cofactor for any element you do not you can define, the cofactor for this element also.

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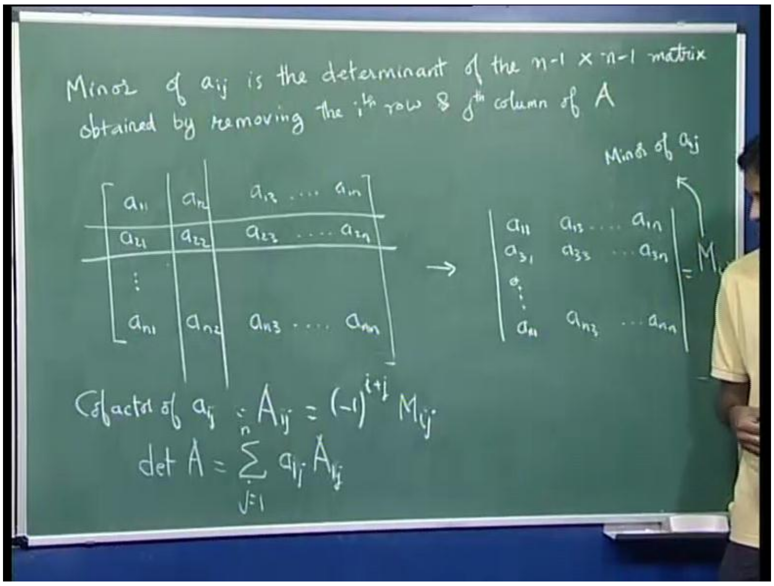

So, when you define the cofactor of a 12, we preserve the order now there is another quantity called the minor so minor of a ij is the determinant of then minus 1 by n minus 1 matrix obtained by removing the ith row and jth column of a. So, if this matrix a has elements given by a ij then you can define the minor of any element as the determinant of the n minus 1 by n minus 1 matrix obtained by removing the ith row and jth column of a.

So, suppose you have a matrix a 11 a 1n a 21 a 223 a 2n all the way up to a n 1 a nn if, you want the calculate of minor of a 22 then what you do is you remove this row, remove this column and you will get matrix a 11 a 13 a 1n a 31 a 33 up to a 3n all the way up to a n1 a n3 up to a nn and the determinant of this matrix is called the minor of i. So this is the minor of a ij, now notice that when we calculated the determinant it is not the minor but it is sometimes the minor appears as it is so if you take what multiplies a 11 is the minor of a 11 but what multiplies a 12 is not the minor. But, In fact, the negative of minor and what multiplies a 13 is the minor of a 13.

So this quantity which is sometimes equal to the minor and sometimes equal to the negative of the minor is called the cofactor. So, cofactor of a ij and this is denoted by a. So this is denoted by a ij capital A ij and this is equal to minus 1 raise to i plus j a ij or m ij. So it is minus 1 raise to i plus j of m ij so the cofactor is related to the minus when, the simple relation and now. Now we can write the determinant of a is nothing but the some of the elements of each of the row times the cofactor of those elements. So, it is nothing but some over j equal to 1 to n a ij times cofactor of ij or a 1j. So, you can take the first row so I have used the first row for the calculation of the determinant and actually, I can take any row, I do not need to take the first row.

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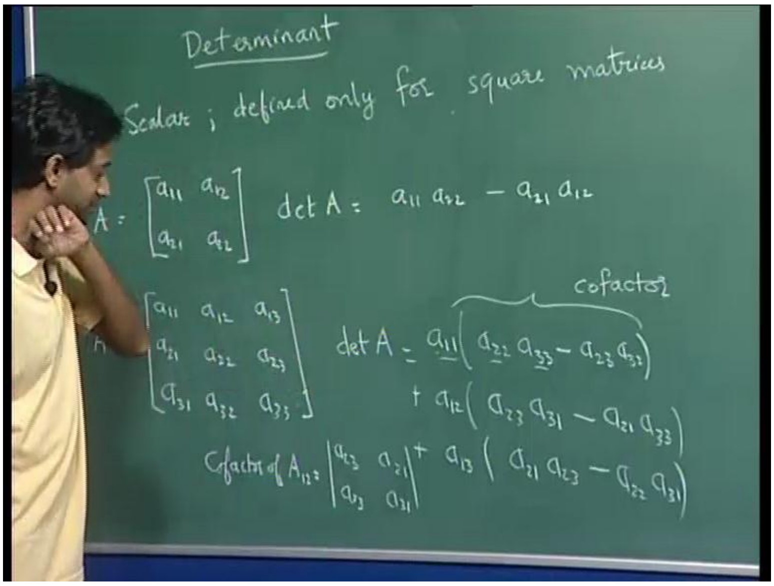

I can use the, I can calculate the determinant using the second row or the third row or any other row and also you need not use rows, you can also use column. So, I can use a first column, I take the sum of elements multiplied by their cofactors, some of element of a 21 multiplied by cofactor of a 21, some of and then a 3 times cofactor of a 31. So, I can do it even column wise or row wise and this is very useful because sometime it is fastest to calculate a determinant using some particular row or column.

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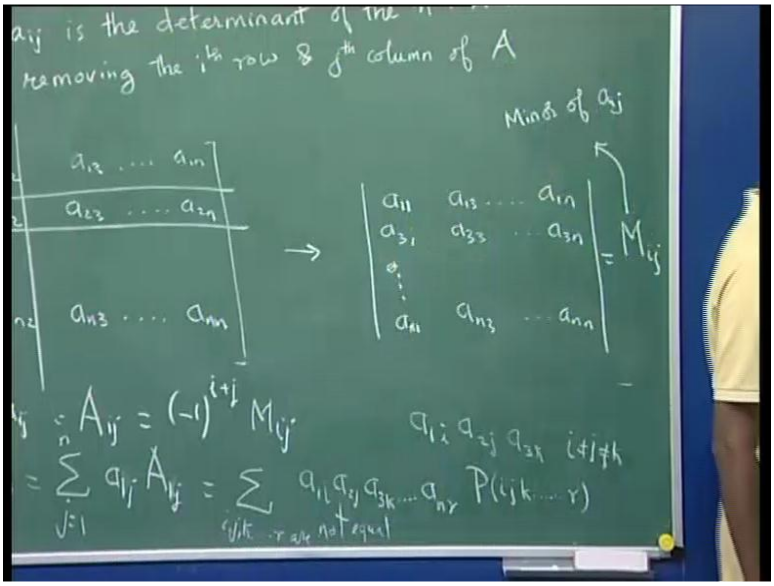

So, the cofactor turns out to be a very useful way and this definition of the determinant is what is the useful definition of determinants, especially when you are dealing with matrices of a very high order. Now a thing to note is that each term in the determinant if, you look at the various terms, this is a 11 a 22 a 33 any how a 1 a 23 a 32 so each term and the and then if, you look at this term a 12 a 23 a 31 a 12 a 21 a 33. So each term in the determinant has a form so each term in the determinant looks like a 1 and some element, some element I will say I a 2, second row and some element j, which is not equal to I, and then a 3k, where k is not equal to i or j.

So notice that each element has this form where it is it looks like a 1i a 2j a 3k where, i is not equal to j not equal to k. So, i j k are all distinct, so i is not equal to j i is not equal to k, and j is not equal to k so each term each element looks like this and so the determinant looks like a sum of terms of that form and but some of them have a positive sign and some of them have a negative sign and this inspires another way of writing the determinant as a sum of various terms of the form a 1i a 2j a 3k and so on. Up to if, you a n by n matrix, then it is n j k l i will just call it nr so where i j k extra r not equal to each other. So each of them are distinct and you sum over all possible such combinations and there is an index sometimes it is plus minus. So there is a factor called. I will write it here it is called.

So, you multiply this by P of i j k up to r so you sum over all possible terms of this form but sometimes P is plus 1 sometimes P is minus 1 and this P is called the permutation index and this permutation index can be plus or minus 1. So this permutation index is plus or minus 1 and it is equal to plus 1 then you call it an even permutation if, it is equal to minus 1 you call it an odd permutation.

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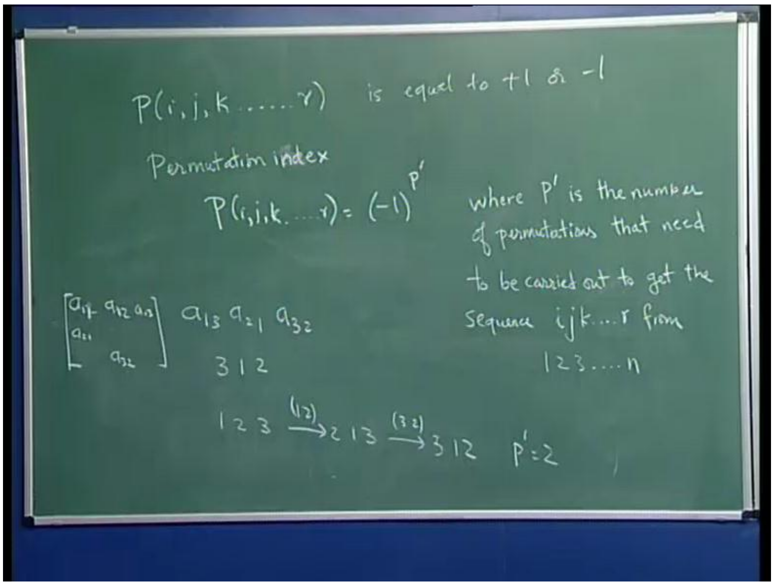

So P of I jk up to r is equal to plus 1 or minus 1 and this is called the permutation n index and sometimes this is written as P is equal to minus 1 raise to pi will call this P prime where, P prime is the number of permutations that need to be carried out to get the sequence i j k up to r from 1 2 3 to n. So what this means is suppose, you have a term in the determinant that looks like a 13 a 21 a 3 a 32 suppose, you have a term that looks like this then this sequence i j k up to r, is basically 3 1 2 and now you have to see how many permutations you have to do to get 3 1 2 from 1 2 3, so we start with 1 2 3.

Now if, i switch 1 and 2, so first I switch 1 2 then I get 2 1 3 then I switch 3 2 then I get 3 3 1 2 therefore, I have to do 2 switches so P. So, P prime equal to 2 so P prime equal to 2 means, you have minus 1 square that is plus 1. So, this term will appear with a plus sign in the determinant and you can easily verify this because this term is if, we take a 3 by 3 determinant or 3 by 3 matrix a 1 3. So, this is this term multiplied by a 21 into a 32 and clearly this should appear with a positive sign and you can verify that because P prime is 2 minus 1 raise to P prime is plus 1 and therefore, this permutation will appear with a plus sign.

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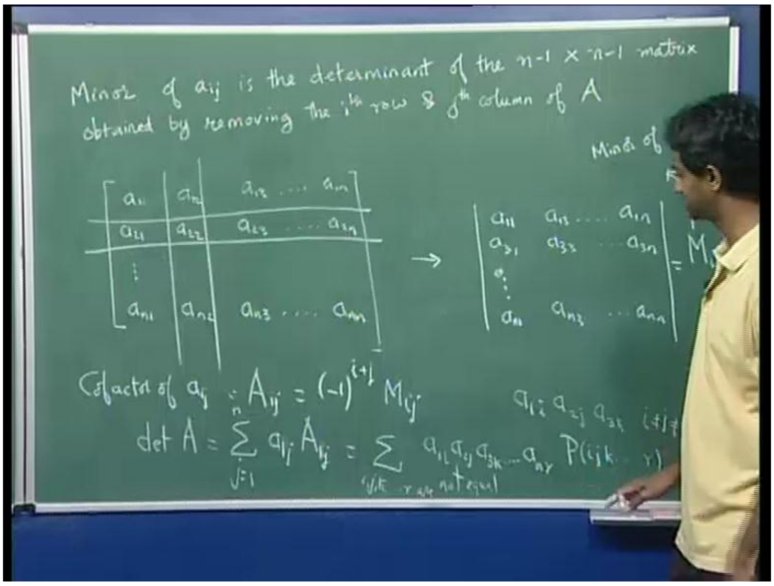

So this permutation methods works is another way of calculating the determinant of a matrix and typically when, we were dealing with large matrices then some of these methods are quite useful however. It is it might be fairly interesting and intriguing for you to know that if, you are calculating the determinant of a large matrix and when, I say large I mean greater than 10, I mean 10 is also a large enough. But, any matrix larger than 10 then it turns out that this way of calculating the determinant using cofactors minus turns out to be much less efficient than a method of Gauss elimination. So, that is something that you should know when, ever you are numerically calculating the determinant of a large matrix. Then it is always better to use Gauss elimination now why is Gauss elimination useful for calculating the determinant.

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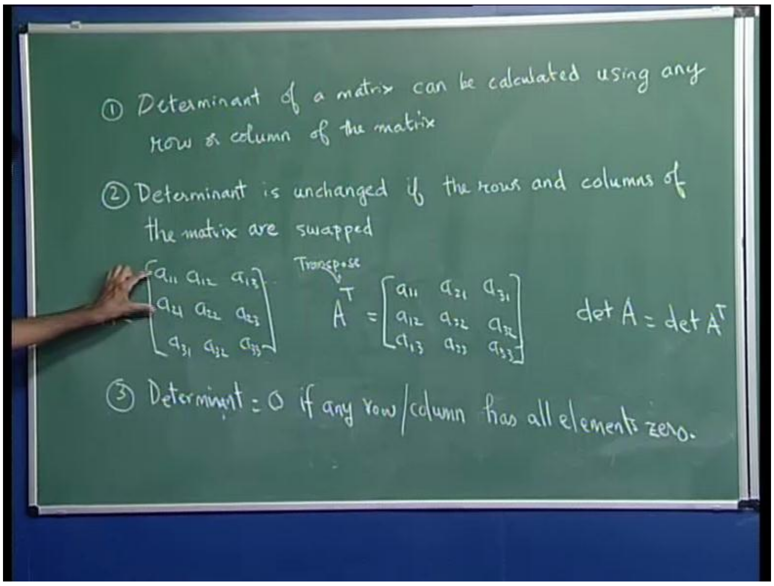

So, in order to see why Gauss elimination is useful for calculating the determination of matrices let us, write down a few properties of determinants. So, the first 1 is you can calculate, so determinants of a matrix can be calculated using any row or column of the matrix. So, in the examples that we looked, so far we were always using the top row or top column but you can calculate a determinant using any row or column next is and this it follows from the definition of the determinant that the determinant is unchanged if, the rows and columns of the matrix are swapped. So, in other words if, I had a matrix that looked like a 11 a 12 a 13 let us just take a 3 by 3 matrix a 21 a 22 a 23 a 31 a 32 a 33.

Now, if I change the rows into columns and columns into rows than the matrix I get is called a transpose so this matrix is called a transpose and this is given by a 11. Now instead of a 12, I put a 2121 a 31 and then and what, I have done is I have instead of putting a 21 here. I will put a 12 here, a 22 will remain the same, so I have a 12 a 22 a 32 and then I have a 13 a 23 a 33. So this matrix is called a transpose notice that we have interchanged the off diagonal elements but the diagonal elements are unchanged and it turns out that determinant of a equal to determinant of a transpose.

So determinant is unchanged if, the rows and columns of the matrix are swapped the third property is that determinant equal to 0. If, any row slash column contains each element to be 0 so a determinant of matrix is 0 if, any row of row or column contains each element of each element 0 contains as all elements 0. So, if I have and this is very obvious to see if, I have 0 if, I have any 1 row or column to be 0 then I can always calculate the determinant using that particular row or column and I can. So, if I have the column as 0 I would calculate the determinant using this column and so I would multiply this by the it is cofactors so and then this by it is cofactor and this by it is cofactor and since each of these are 0, the determinant will be 0.

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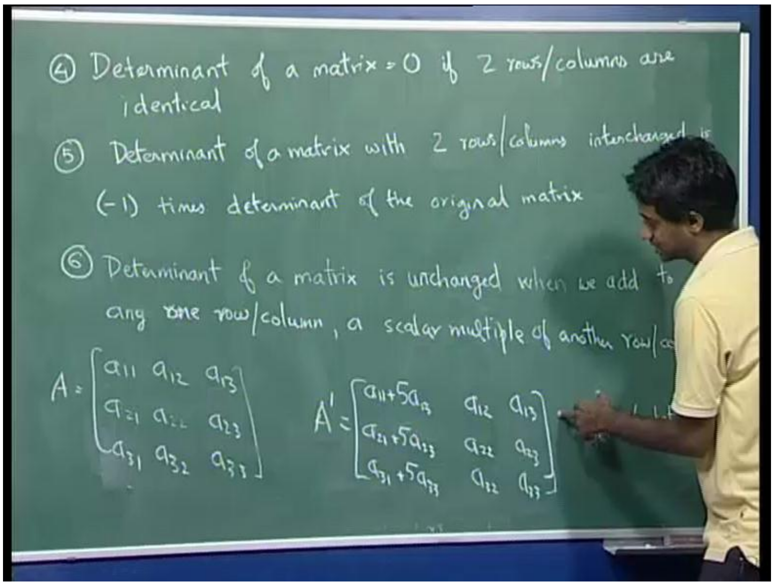

Know the next property is probably the most useful property of the determinant and this is that determinant of a matrix equal to 0 if, 2 rows slash columns are identical. So if any 2 rows or columns are identical then the determinant of the matrix is 0. So, and that is also fairly obvious to see because suppose let say these 2 columns where, identical is these 2 columns are identical then I can always calculate the determinant using this column and the cofactor each of the cofactors will be 0. So, if these 2 columns are identical then the cofactors will be cofactors of elements of this row this column will be 0. So, the determinant of a matrix is 0.

If 2 rows or columns are identical next determinant of a matrix with 2 rows or columns interchange is minus 1 times determinant of the original matrix. So, suppose I take a matrix a and i calculate it is determinant then let us say, i swap 2 rows i or I, swap 2 columns of a then the determinant of the resulting matrix will be negative 1 of the determinant of a and the last property that that follows from the from this property is that determinant of a matrix is unchanged when, we add to any 1 row or column as scalar multiple of another row slash column.

So what i mean is suppose, I have a matrix a, which is like this now to each element in a i add a scalar multiple of some other row. So, for so if I have a is equal to 3 and if, I have a prime. So, I take lets say to the first column i add 5 times the 3 column a 13 a 21 plus 5 a 23 a 31 plus 5 a 33 and I have a 12 a 13 a 22 a 23 a 32 a 33. So, basically I kept everything else same but to 1 row i added a scalar multiple of another row then the determinant of a prime equal to determinant of a. So the determinant of a prime is equal to determinant of at here are some other properties of determinant suppose, I take a determinant of a some of matrices.

So, if I construct 2 matrices of the form so the reason why this is true is that the determinant has the property that the, determinant of this matrix a is equal to the determinant of a matrix, where you just a 11 a 21 and a 31 here plus a determinant of a matrix where, you just where you just put this term. So this gives us this is another property of the determinant and it is important to be a little careful here.

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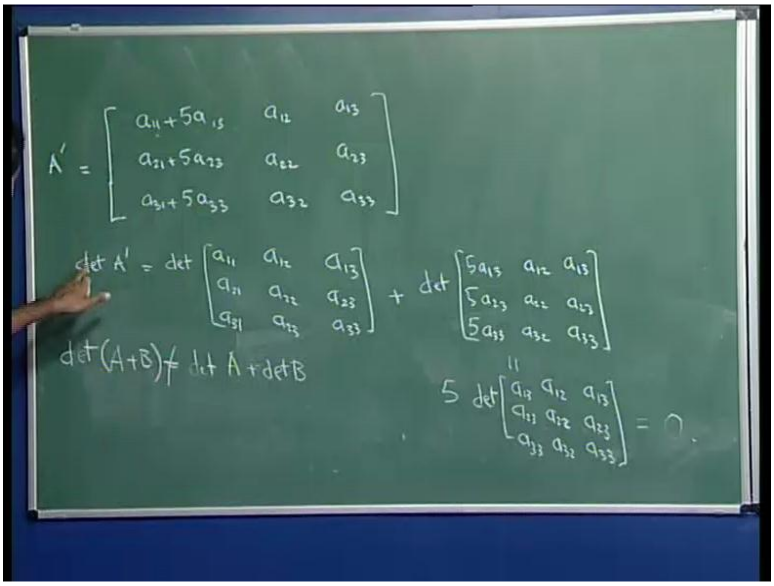

So, suppose I have a 11 plus 5 a 13 a 21 plus 5 a 23 a 31 plus 5 a 12 a 13 a 22 a 23 a 32 and I will call this a prime. So, the property of the determinant is that the determinant of a prime is equal to the determinant of an a 22 other interesting properties of determinants. Now the determinant of this matrix a prime is equal to determinant of this matrix where, whenever you have something like this, where you have sum of terms, you can write this in this form. So, determinant prime is the determinant of this matrix which, is just a plus determinant of so you had this plus this.

So, this is the property of the determinant that if, you add an elements if add elements to 1 row then you can split the determinant into these parts, then you can add the determinants now remember determinant of a plus b, if you add up 2 matrices. The determinants of the sum is not determinants. So, if you add up matrix a plus b then determinant of a plus b is not equal to determinant of a plus determinant of b. So, this is not true however, you if you just add elements to 1 row then the determinants can be added in this form the other property is that the determinant of this matrix is equal to. So, whenever you add 1 elements of 1 row you multiply it by a scalar.

Then the determinant gets multiplied by the scalar. So, 5 times determinant of a 13 a 23 a 22 a 23 a 33 a 32 a 33. So, whenever you multiply all the elements of 1 row or a column by a scalar then the determinant of the whole matrix gets multiplied by that scalar. So, determinant of this matrix is 5 times determinant of this matrix without the scalar now the determinant of this matrix because 2 rows or columns are identical.

So, in this case the first column and the 3 column are identical. So, the determinant of this matrix is 0 and therefore, this whole part is 0 and so determinant of a prime becomes equal to determinant of a. So, in the next class we will how we use determinants in where, they appear in the solution of a system of linear equations.