Mathematics for Chemistry
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Lecture - 11

We have looked at determinants and we have looked at various properties of determinants, now determinants when we are looking at solutions of linear equations.

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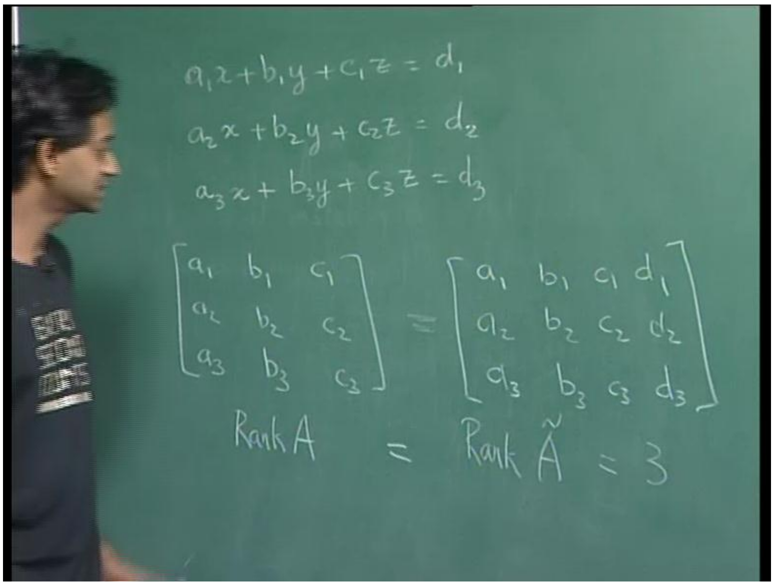

So, suppose you have a set of 3 linear equations of the form a 1 x plus b 1 y equal to d 1 and I am taking 3, but I can extend it to any number of equations. So, suppose you have a linear equations, now we already saw that the condition for these equations to have a solution to have a unique solution is that the rank of the matrix formed by a 1 a 2 a 3 b 1 b 2 b 3 c 1 c 2 c 3, the rank of this matrix has to be equal to the rank of this matrix. So, rank of A we call this matrix A and this is the augmented matrix A tilde.

So, rank of a has to equal rank of A tilde, and this has to equal the number of independent variables that is 3. So, if the rank of this matrix is equal to the rank of the augmented matrix and that is equal to 3, then this set of equations has a unique solution and now you can show by simple algebraic manipulations.

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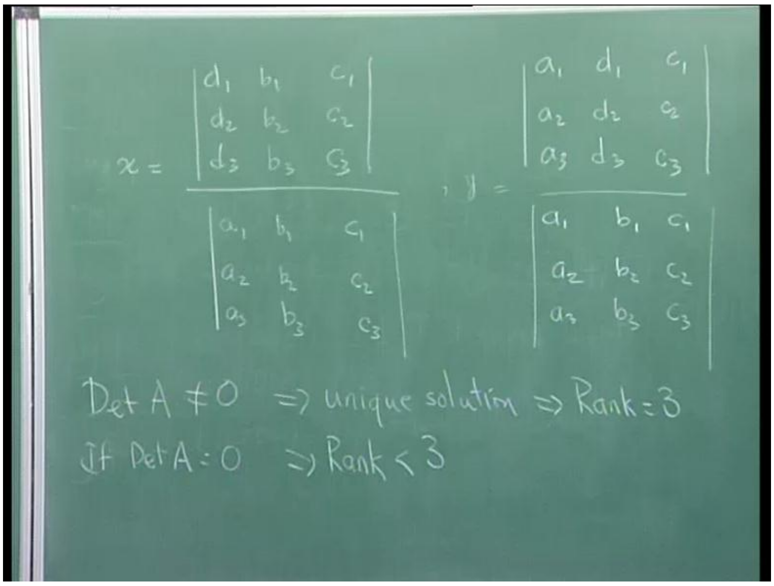

That this solution is given by x is equal to ratio of determinants and the determinant at the bottom is always a 1 a 2 a 3 b 1 b 2 b 3 c 1 c 2 c 3, and if you want to determine the first variable x, then you replace the column a 1 a 2 3 by d 1 d 2 d 3. And you get a matrix d 3 b 1 b 2 and x turns out to be equal to this and you can show this by fairly straight forward algebraic manipulations, similarly y is equal to...

So, the denominator is a same but the numerator now, you leave the first row as it is and you replace the second row by d 3 and leave the third row as it is similarly, when can write for z also similarly, for z. So, we notice that in the solution of the of this linear equations determinants appear very naturally and this can be extended to solution of more equation even, you do not need to have 3 equations for any number of equations you can use the same procedure to calculate the values of the variables. Now a thing you notice is that the determinant that appears in the denominator is a same and this determinant is the determinant of A.

So it is the determinant of matrix A and this determinant cannot be 0 because the solution has the determinant in the denominator. So determinant A not equal to 0 and it is not hard to show that if, determinant A is not equal to 0 then this implies unique solution and actually this is also a way to check the rank of this matrix. So, implies A rank equal to 3.

So, if the rank of A is 3 then the determinant of A is not equal to 0 and vise versa if, the determinant of A is not equal to 0, the rank is equal to 3. So the condition for unique solution to exist is that this determinant should not be equal to 0 or in other words the rank should be 3 and now it follows that if, determinant a equal to 0 then rank less than 3, rank has to be either 2 or 1, if determinant A is 0 and vice versa. So, the determinant is intimately connected to the rank and A way to check a way to the rank of some matrix is to calculate the determinant and see if, the determinant is 0 then the rank is less than 3 if, the determinant is not equal to 0, the rank is equal to 3.

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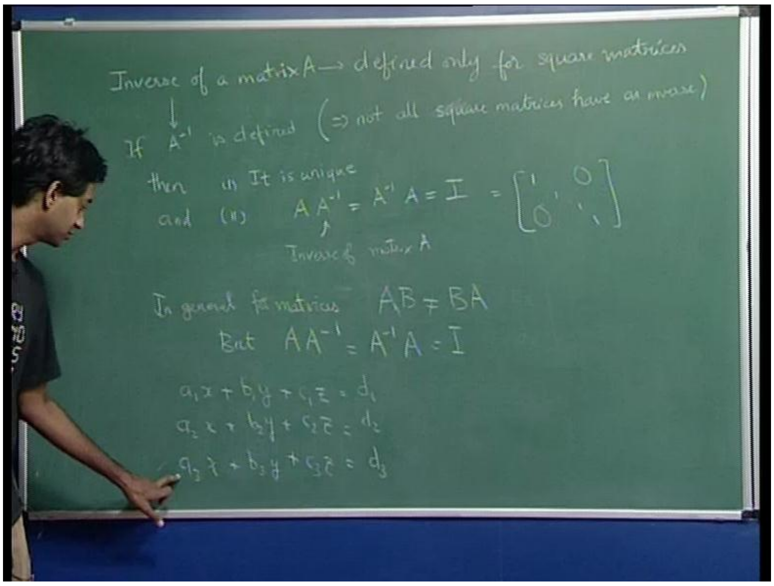

The next concept that we will discuss is that of the inverse of a matrix. So, the inverse of a matrix and like the determinant, it is defined only for squares matrices. So it is defined only for square matrices, now the inverse of a matrix if it is defined. So, if A inverse is defined that means not all matrices have an inverse so this directly implies that not all matrices not all square matrices have an inverse. So, this is important to keep in mind if it is defined 2 things first 1, it is unique and second thing A inverse A equal to identity so if a matrix is if a, if you have a matrix at the inverse of a matrix, we call this matrix a if, you have a matrix a then it is inverse is denoted by A.

Inverse and it is unique and a inverse satisfies, a inverse equal to a inverse A is this is inverse of matrix A and this inverse of a matrix A is also a matrix it is also a matrix and when, and it when it multiplies a then you get the identity matrix that is 1 along the diagonals and 0 in the of diagonals. So, if a is a 3 by 3 matrix then a inverse is also a 3 by 3 matrix and their product gives a the identity matrix the 3 by 3 identity matrix. However, if a is a larger matrix then a inverse will also be a matrix of the same size and identity matrix will be the identity matrix of the lagers size, now remember in general for matrices a times b is not equal to b times a. So, in general this is not true it may be true in some special cases.

But, a inverse equal to A inverse A and the product is nothing but the identity so in other words the multiplication of A and A inverse is a commutative operation so A inverse is same as a inverse A. It is not true in general for matrices but in this case it is true so this is the definition of the inverse of a matrix and now, why is the idea of inverse of a matrix useful and to do this we look at again.

We had the system of equations and we can we had the system of equations a 1 x plus b 1 y plus c 1 z equal to d 1, a 2 x plus b 2 y plus c 2 z equal to d 2, and a 3 x plus b 3 y plus c 3 z equal to d 3, and now if we define.

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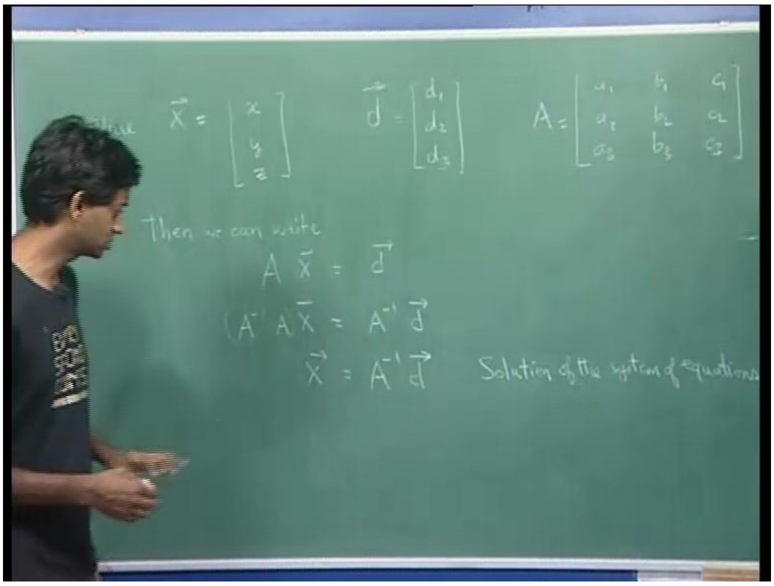

So, define X vector is equal to x y z, D vector is equal to d 1 d 2 d 3 and A matrix. A is a matrix a 1 a 2 a 3 b 1 b 2 b 3 c 1 c 2 c 3. Then we can write these 3 equations in a simplified form A times X equal to D, so this set of 3 equations can be written in this form and we have already seen this. Now suppose, I multiply on both sides by A inverse. So, suppose I take this and multiply on this side by A inverse. So, I will get a inverse A

X is equal to a inverse D and then you use the fact that a inverse, A is nothing but the identity.

So, you perform this multiplication first. So, you get X equal to A inverse multiplied by D. So, what that means, is that if you know the inverse of A then you can easily calculate, you can easy solve this system of equations. So, this is a system of equations and the goal is to solve for x y and z in other words the goal is to solve for X inverse for for X vector and if, you know the inverse then the solution is very straight forward, you just multiply D by X to get by A inverse to get the solution. So this is the solution of the equations, so the massage is that if, you know the inverse of this matrix a then you can then you know how to solve this system of equations, so the inverse is also related to the solution of the set of equations.

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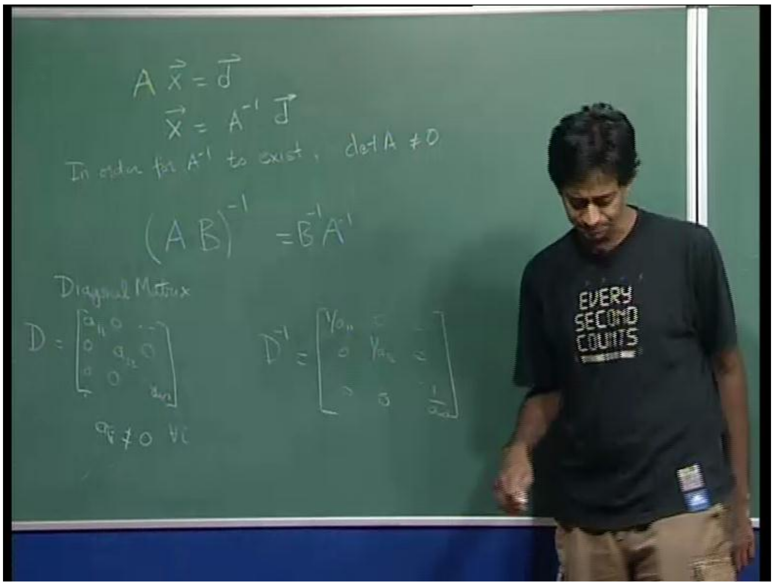

Now we already said that for a system of equations to have a unique solution the determinant should not be equal to 0, the determinate of the corresponding matrix should not be equal to 0. So, we said that suppose you had we had a times X equal to D then the condition for unique solution, so to solve for X was our matrix x y z and the condition to get unique values of x y z was that this, the determinant of this matrix should not be equal to 0. Now we also wrote that is equal to a inverse multiplied by D so what does this imply about the inverse.

So what this implies is that in order for a inverse to exist determinant a has to be different from 0 so if the determinant of a is 0 then the inverse of a does not exist and this makes it consistent with the idea that if, you if the determinant a was equal to 0 then this is set of equations does not have a unique solution and in other words you cannot write this in this unique form and I should mention right here.

That this very step when you solve a set of equations using matrix methods by using the inverse it is the single largest application of matrices in various engineering and chemistry applications. So, often you set up your problem in a way that you have a large number of equations and you set it up in matrix form and your goal is to invert the matrix and find the solution. Now we can look up some simple properties of inverses suppose, have a matrix a and a matrix b and you take the product of these 2, what is the inverse of the product of this these two.

And clearly it is equal to B inverse A inverse and you can verify this because if I take B inverse A inverse and multiply it by a B then you show that you get the identity matrix. So the inverse of a product of matrices is the product of the inverses taken in the reverse order. Now next suppose, you had a matrix that was diagonal, so a diagonal matrix so that means, you have let us say a 11 a 22 along the diagonals and all the of diagonal elements are 0.

So, all these of diagonal elements are 0. So, if we add a matrix like this then you can show that the inverse of this matrix so if I call this matrix D for diagonal matrix is this then you can show that D inverse is equal to is also a diagonal matrix. But, the elements that appear here will be 1 by a 11 by a 22 by a n n as a n n and it is 0, in the of diagonal elements and you can show this because if you multiply these 2 matrices you multiply this row with this column.

So, you so a 11 into 1 by a 11 that will give you 1 and everything else will be 0 and you can show similarly, that when you multiply by all these rows with all these columns you will just get 1 along the diagonals. So, the determinant so the inverse of a diagonal matrix is also a diagonal matrix, but the elements on the diagonal are the reciprocal of the elements along the diagonal of the original matrix and this also implies that a ii cannot be 0.

So, none of the elements are 0 so for all iso none of these elements can be equal to 0 so in other words none of the diagonal elements can be equal to 0 because if any of these are 0, then the 1 over that element is not defined. So diagonal matrix is very easy to calculate the inverse and so now this tells us the strategy for.

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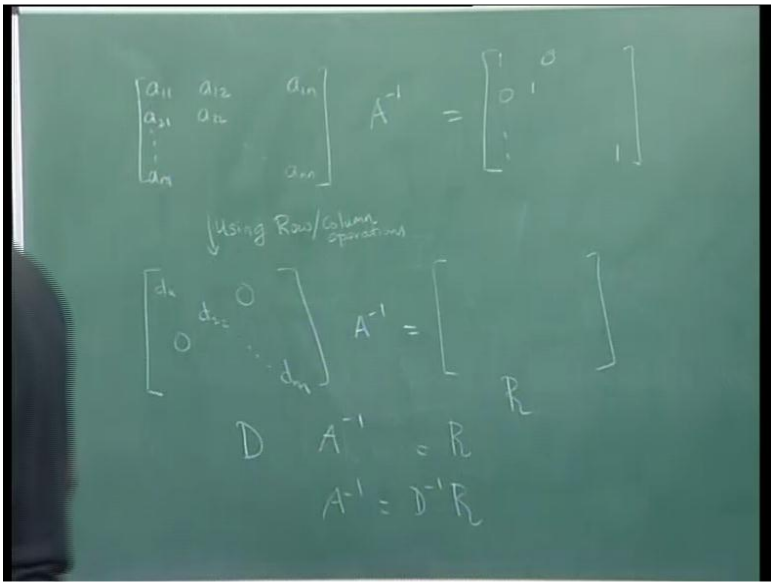

Calculating the inverse of a matrix this the idea that a diagonal matrix is easy to invert gives us a strategy for calculating the inverse of any matrix and that is a following. So, suppose if, you had a matrix of this form a 11 a 12 a 1n a 21 up to a n1 all the way up to a nn. So we say that a times inverse equal to identity matrix, so this is equal to the identity matrix and what 1 can do is 1 can do a set of row and a column operations and you convert this to a diagonal matrix and we do exactly the same set of row and column operations on this matrix so on.

The identity matrix so you do a set of row and column operations to convert this in to a diagonal matrix. So, you do by various row operations row and column operations you convert this to diagonal form and you convert it to some you finally, might end up with d 11 and 0s. Everywhere else, equal to now you are going to do the same set of operations on the identity matrix. So, you will get some other matrix, which is not necessarily diagonal or anything like that and once you have this.

Now you can multiply on both sides by D inverse, so this matrix is D times a inverse and let me call this matrix R the this is the result of doing all these operations on the identity matrix then you can now d inverse is very easy to calculate. So then you can just say that a inverse equal to D inverse R so by using this row and column operations you can calculate the inverse of a matrix, now in addition to this there is also a simple.

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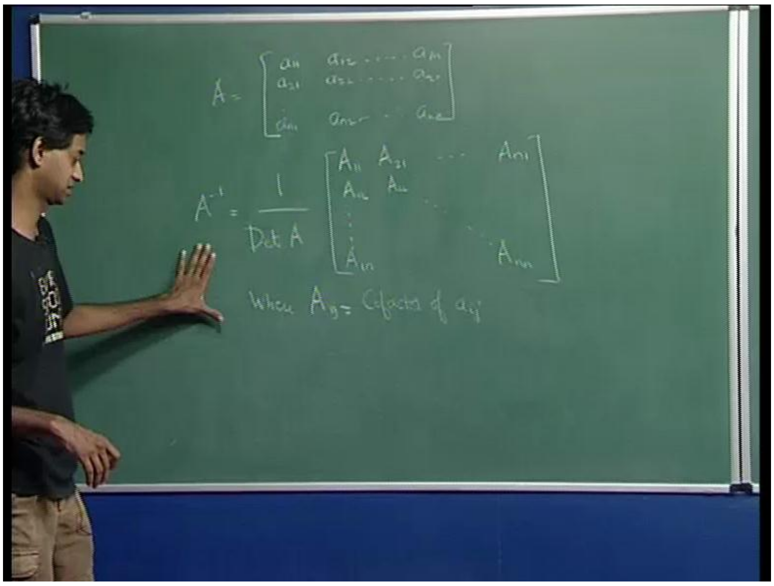

Formula for calculating the inverse that is what we will discuss next, so the inverse of this matrix. So, if I call if I say A is equal to a 11 a 121n a 21 a 22 a 2 n a n1 a n 2 a nn then you can show that a inverse is equal to 1 by determinant of A and you get a matrix and the matrix you get here is the following you get capital A11nn and then at the of diagonals you get capital A of 2 1 in here you get capital A of 1 2 in all the way up to capital A of n 1 and here, you get capital A of 1 n notice the element of the inverse corresponds to capital a of 1 1n.

So, capital A of 1 n not n 1 where, a I j equal to cofactor of a i j, we already defined what the cofactor is so a i. So, capital a i j is the cofactor of a i j. So, for example, if you want to calculate the cofactor of a to 1 then you delete this row and this column and the resulting matrix that you get.

You take the determinant of that matrix so that is the cofactor with the appropriate sign which, will be plus or minus 1. So, if you know the cofactors of each of these elements then you can calculate the inverse of a matrix now in order to calculate the cofactors you need to calculate the determinant of an n minus 1 by n minus 1 matrix.

So we need to calculate the determinant of a and then for each of the cofactors you need to calculate the determinant of a of an n minus 1 by n minus 1 matrix, and it is found that numerically for large matrices this procedure is not very efficient so if you want to invert large matrices, then this procedure turns out to be hugely inefficient where, as it is much easier to use procedure like this where you keep doing row and column operations and to convert a to a diagonal matrix.

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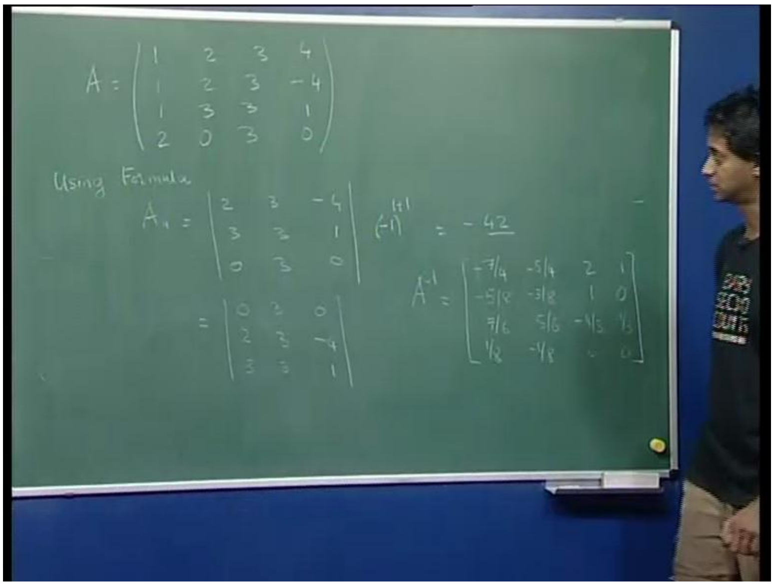

Next we look at the example, of the calculation of the inverse. So, I let my matrix be A is equal to 3 4 1 2 3 minus 4 1 3 3 1 2 0 3 3 0. So this is my matrix A and you are asked to calculate the inverse of this matrix, so let us try to do it using both the methods. So, first let us use the formula. So, using formula so in order to use a formula you need to calculate the determinant of A and you need to calculate the determinant of each of these cofactors. Now let us try to calculate the determinant of A, I mean that is that is going to be a long procedure but when you do that procedure and you calculate both the determinant of a and each of the cofactors of a you will get the inverse.

So, what I will do here is I will look at the cofactors 1 by 1. So, let us calculate the cofactor of the first element. So, the cofactor of this element is denoted by A 11 and this is equal to the determinant found by of the matrix found by deleting the rows and columns so if you delete these rows and columns then you get the matrix 2 3 minus 4 3 3

1 0 3 0 so you get this matrix and it is the determinant of this matrix multiplied by minus 1 raise to this is 11.

So, it is 1 plus 11 plus 1 is 2 and you can show this that this is equal to 2 times well I think easiest is to use this row if, you bring this row on top then you can calculate the determinant using this row. So this is equal to determinant of 0 3 0 2 3 minus 4 3 3 1 by cyclically permitting the rows then I do not change the determinant so then I can use this row and I can calculate the determinant as 3 into minus 4 into 3 is minus 12 minus 2 into 1. So, minus 14 3 into minus 14 is minus 42.

So the into 3 is minus 42 and now you can go head and you can calculate each of the other cofactors so you have to go step by set and calculate each of the other cofactors and if you go head and go through that procedure, you will get that A inverse. So, if you go through this procedure 1 by 1, like I showed you how to calculate this cofactor then you have to go head and calculate the cofactors of each of the 16 elements and when you do that process, what you will get is that A inverse is equal to and you go through that procedure and also and after that you divide by the determinant of this matrix. Then the answer turns out to be minus 5 by 4 2 1 minus 5 by 8 1 0 7 by 6 5 by 6 and finally, 1 by 8 0 0. So that is the determinant of this matrix.

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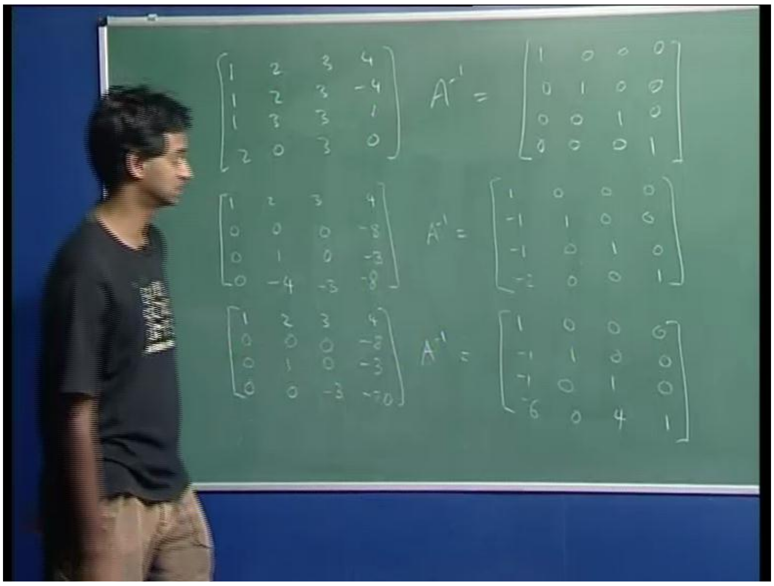

And you can get this by using this formula next let us, see how we will do it using the method of Gauss elimination. So in order to use Gauss elimination what we have to write is 1 2 3 4 1 2 3 minus 4 1 3 3 1 2 0 3 0 a inverse equal to identity matrix. So, this is the basic formula that we start with and now what we want to do is to convert this to a diagonal matrix using row operations.

So, the first operation you will do is you want to convert this 1 to 0. So, you subtract this row from this row. So, when you do that you get 1 2 3 4 and when you subtract this row from this row, you will get 0 0 0 minus 8. Next you want to convert this to 0. So, you subtract this row from this row so you get 0 3 minus 2 is 1 3 minus 3 is 0 1 minus 4 is minus 3 and you subtract twice this row from this row.

So, you get 0 2 times, 2 is minus 4. So, 0 minus 4 is minus 4 3 minus 6 minus 3 0 minus 8 minus 8 and this times a inverse is equal to a matrix on the right. Now what we did is from this row we have to subtract this row. So, you get minus 1 1 0 0 and you subtract again you subtract this row. So, you get minus 1 0 1 0 and from this row you subtract twice this row. So, you get minus 2 0 0 1. Next what we want to do is 2 make this element 0.

So, in order to make this element 0 you have to subtract this but unfortunately this is 0 so we cannot use this row to subtract this row to eliminate this element so let us go ahead and try to convert this to 0. So, if you want to convert this element to 0 then what if you want to convert this element to 0 what you will do is you will add 4 times this row. So, if you do that then so you get 0. So, when you add 4 times this row you will get 0 here 4 times this row you will get 0, 4 times this you will get minus 3 minus 8 plus 4 into minus 3.

So, minus 8 minus 12 minus 20 so this way you can go ahead and you can convert this element to 0. Now the same thing has to be done on this side to. So, this to so here you have not touched any of these elements but now you subtracted or you added 4 times this row. So, minus 2 minus 4, so that becomes minus 6 0 4 1 then again you find that, you cannot convert this to 0, using this row so then our next strategy is to try to convert this element to 0, using the row below so we convert this to 0, using the row below and that will ensure that these elements are not affected. So, you go ahead you will convert this row to 0 using this row.

So, what we do next is to convert all the terms on the upper diagonal to 0 and to do that you start with this so if you want to convert this to 0, you multiply this row by 20 this row by 3 and you subtract the 2 row. So, when I multiply this row by 20, I will get minus 60 and I subtract 3 times this row. So, I will get 0 here when I multiply this by 20, I will get 0 and I subtract 3 times this. So, 3 times minus 3 is 9 3 times minus 3 is minus 9. So, 0 minus 9 is plus 9. Similarly, when I multiply this by 20, I will get 20 and minus 0 is 20.

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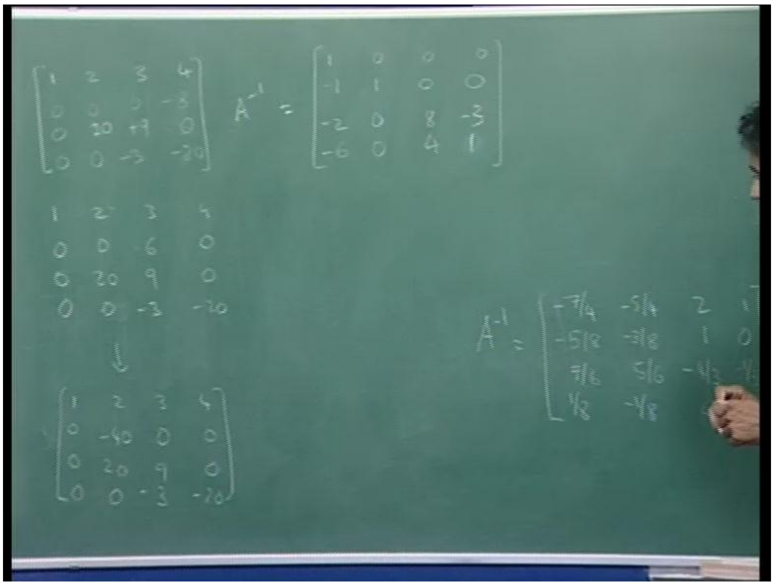

So that is what I will get. So, this times A inverse is equal to 1 0 0 0 minus 1 1 0 0 minus 6 0 4 0 and then and what I will get here is 20 times this. So, 20 times minus 1 is minus 20 and plus 6 times 3 18. So, that is minus 2 and here, it will be 0 because both were 0s in this case 20 times, 1 is 20 minus 12 is 8 and in this case the 1, I had minus 3 so you go through this procedure.

I mean I would not go through all the details but you then you convert each of these elements to 0 till you finally, get a diagonal matrix you we still have to convert, now we can convert this element to 0 or it is better to convert this to 0. So, if you want to convert this to 0, then you will do 1 2 3 4, so to convert this to 0, you multiply this row by 5 and subtract this row into 2. So, you will get 0.

So, this row this into 5 is 0 plus 6 0 0 0. Now I can convert this to 0 using this row so I have to do the same thing on the right. I would not go through this but if I when I convert this to 0 then I will use 3 into this minus 2 into this. So, when I use 3 into this 18 minus 18, I will get 0 this will remain 0, this will give me minus 20 so 1. So, this will be 0 so 2 into this minus 40 0 0 0 and you have to do the corresponding operations here. Now you can convert this element to 0, using this row so when you do this the you do 2 into this plus this then this will be unchanged, this will be unchanged, this will be unchanged.

And only this element will go to 0 then you can convert once this element is 0, you can convert this to 0 and you can go through, this whole procedure till you get a diagonal matrix. So both these methods are fairly straight forward to implement and it turns out that numerically it is the method of this Gauss Jordan elimination which is favored.

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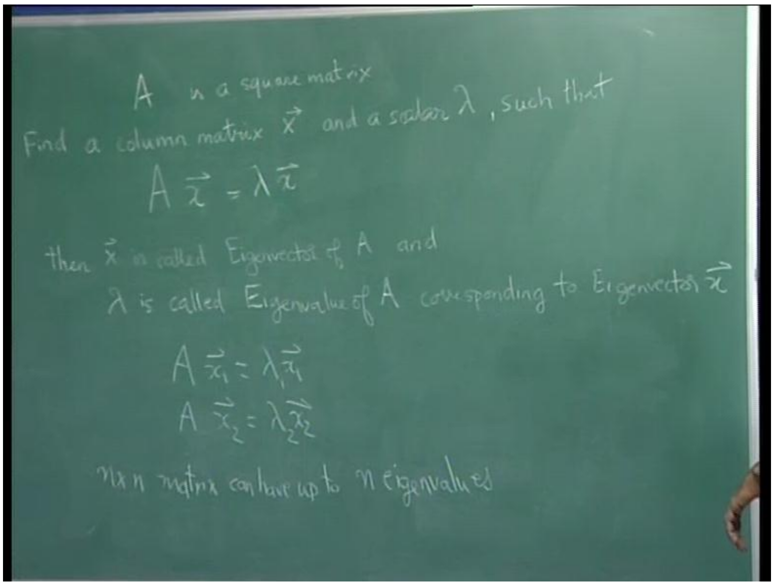

The next concept involving matrices is that of Eigen values and Eigen vectors. So, suppose you have a square matrix A, is a square matrix then there exists so if. So, find a column matrix x and a scalar lambda, such that A times x equal to lambda time x so then x is called Eigen vector of A and lambda is called Eigen value of A. So the import thing about Eigen values and Eigen vectors is that suppose you are A.

Given your given a matrix then there, exists this x and lambda so from a matrix you can calculate both it is Eigen vector and the Eigen value. So and I should emphasize lambda is called Eigen value of a corresponding to Eigen vector x so when you say a x is equal to lambda x then lambda is the Eigen value corresponding to the Eigen vector x. Now in general a matrix has many Eigen values and Eigen vectors many pairs of Eigen values and Eigen vectors and so if you have a matrix it can have many different Eigen values and Eigen vectors. So, you can write a times x 1 is equal to lambda x 1 a times x 2 equal to lambda times x 2 or lambda 1.

X 1 lambda 2 x 2 so these are pairs of Eigen values and Eigen vectors. So, along with an Eigen value you should always have an Eigen vector it is not enough, to say that this is an Eigen value with this Eigen vector it is not an Eigen value for any other Eigen vector. It is an Eigen value only for a Eigen vector x 1 and so on. Now in general if, we have an n by n matrix can have up to n Eigen values and Eigen values and that implies that there are also n Eigen vectors corresponding to these n Eigen values, there are n Eigen vectors. Now we notice we notice that this definition of Eigen values and Eigen vectors has there is something that is not completely specified with respective to the Eigen vector.

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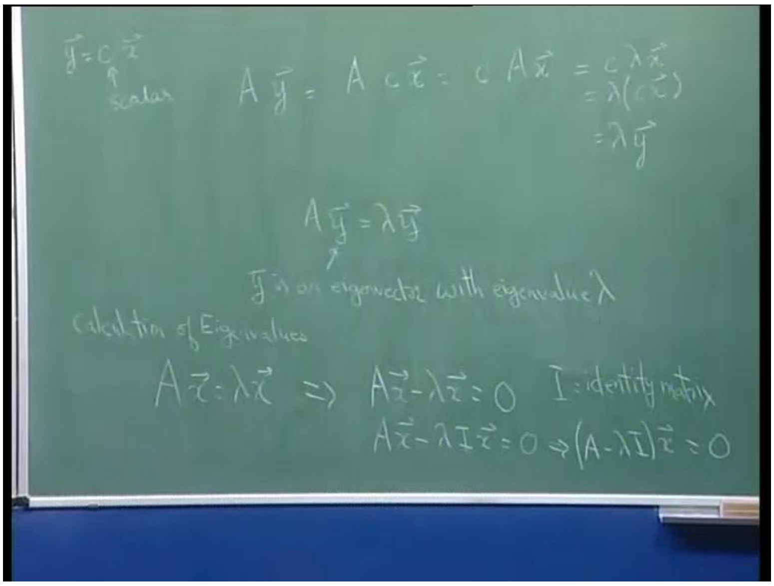

So, in order to see that suppose I multiply x suppose, I say y equal to some scalar times x so y is some scalar multiplied by x then a times y is equal to A times, scalar times x, this is equal to c times A into x. So, this is just multiplying by a scalar and multiplying by a matrix by a scalar is a commutative operation. So, I can switch these and so and what I get is this is equal to c times lambda x, or equal to lambda times c x equal to lambda times y so in other words a y equal to lambda y so that means, y has y is an Eigen vector is with Eigen value lambda.

Now for the same Eigen value you can define you can have infinitely many Eigen vectors. So, by taking different values of c, I can make up infinitely many different Eigen vectors. So, we say that the definition of Eigen vectors is not unique, if you take an Eigen vector you multiply it by a constant you get an Eigen vector with the same Eigen value. So corresponding to an Eigen value you can calculate the Eigen vector up to a constant you cannot, there is no unique Eigen vector but up to a constant you can calculate this Eigen vector.

So, the next thing is how, do we calculate Eigen values and Eigen vectors. So how do we calculate Eigen values and Eigen vectors and in order to do that we start with we will calculation of Eigen values and this procedure is fairly straight forward, what we say is you have a times x equal to lambda x implies a times x minus lambda times x equal to 0 and now I can take write this as a times x minus lambda times i x where, i is the identity matrix equal to 0.

So, i is the identity matrix and this implies that x times a minus lambda i equal to 0. So, this Eigen value equation this is the Eigen value equation and you can write it in this from a minus lambda i times x equal to 0.

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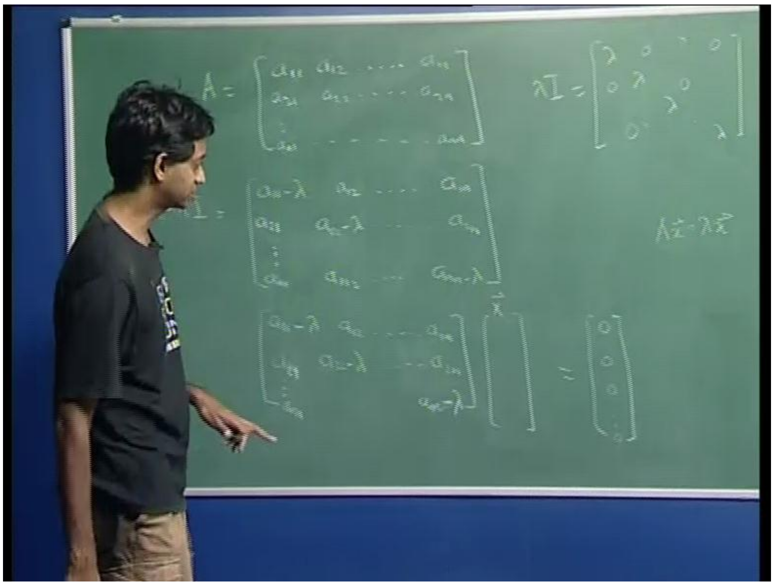

So, how does this help us calculate the Eigen values now suppose, a is equal to a 11 a 12 up to a 1n a 21 a 2 a 2 n and so on up to a 1n up to a nn. So, suppose this is my matrix a then identity is just 1 along the diagonals and 0 of diagonals. So, lambda i the matrix lambda times i is just lambda along the diagonals and 0 for all the of diagonal elements so all the of diagonal elements are 0. So lambda i is that and now if, you subtract these 2 matrices then a minus lambda i is equal to a 11 minus lambda a 12.

Up to a 1n a 21 then a 22 minus lambda a 2n a n1 a n2 a nn minus lambda. So, a minus lambda i is a matrix where, the diagonal elements of a are replaced by the elements minus lambda.

So, you subtract lambda from the diagonal elements and now what you have is this matrix a minus lambda i is this, so a minus lambda i multiplied by x equal to 0. So, you have this expression lambda a 12 all the way up to a 2n and you go a n1 sorry, a 21 up to a nn minus lambda.

So this multiplied by your matrix the vector x is equal to 0. So, we have this expression so a minus lambda x 0 vector and this is the x vector. So, it will contain various elements. So, this is the x vector now, what we have is a system of equations and in this system of equations our right h and side is identically 0. So in this system of equations we find that the right hand side is identically 0.

And this system of equations has a solution where, each of these quantities is 0. So, the trivial solution is that each of these quantities is 0, so if you think of these as the unknowns then the trivial solution is that each of these qualities is 0. But, if there has to be a non-trivial solution, then the determinant of this matrix has to be equal to 0. So, what this means is that if this set of equations has to have a nontrivial solution for these variables nontrivial, I mean all the variables is are not equal to 0, then the determinant this the determinant of this matrix has to be equal to 0.

So, if the determinant of this matrix is not equal to 0, then the only solution is the trivial solution and that is not useful because we know that our Eigen value expression a x equal to lambda x is trivially satisfied by x equal to 0 so we are not interested in the solution where x equal to 0.

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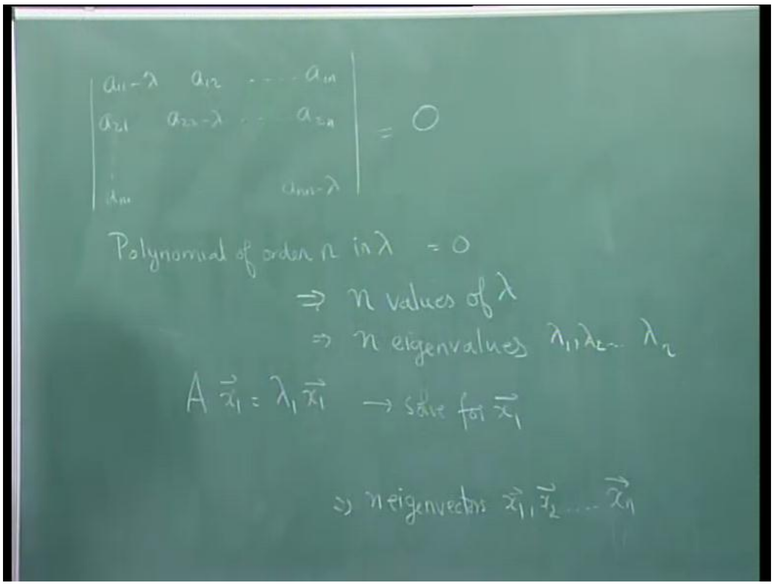

So, in order for nontrivial solutions to exist determinant of that determinant of this matrix is equal to 0 so a 12n a 21 a 22 minus lambda a 2n a n1 a nn minus lambda, this determinant equal to 0 and so this looks like a polynomial of nth order in lambda. So, this is polynomial of order n in lambda so because you have terms like lambda square lambda all the way up to lambda raise to n, and polynomial in order of a lambda n equal to 0 implies n values of lambda.

So, if you solve this polynomial, if you solve this equation then you will get n different values of lambda that satisfy this and so you have n different Eigen values. So this gives me the n Eigen values then if you want to calculate the Eigen vectors, once you have the Eigen values you can calculate the Eigen vectors by substituting, each of these in the Eigen value equations n Eigen values, I will call them lambda 1 up to lambda n. Now, if you want to find the Eigen vectors, then you will say a times x 1 equal to lambda 1 times x 1 and now you can solve this equation for x 1.

So, I have for x 1 x 1 and you repeat for each of the Eigen values. So, we get n Eigen vectors x 1 x 2 x n. So, this is the procedure for solving the Eigen values and Eigen vectors of any matrix, so in the next class we will look at certain special matrices which I will be, which are called as orthogonal hermitian and unitary matrices.

So, this is all you can practice various problems involving Eigen values and Eigen vectors and calculating matrix inverse and so on. So, you refer to any of the text books and you can do a lot of practice problems but in the next class we will go to discussion of various special matrices, which are called as orthogonal matrices then we will talk about hermitian matrices and unitary matrices.