Computational Chemistry & Classical Molecular Dynamics

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Lecture – 16
Errors in Interpolation, Matrix Operations

Hello and welcome to this todays session of our course on computational methods. So, before I go to the matrices, which I am going to describe today, let us summarize what we did in the last 2 lectures. What we did in the last 2 lectures, we listed a large number of numerical methods.

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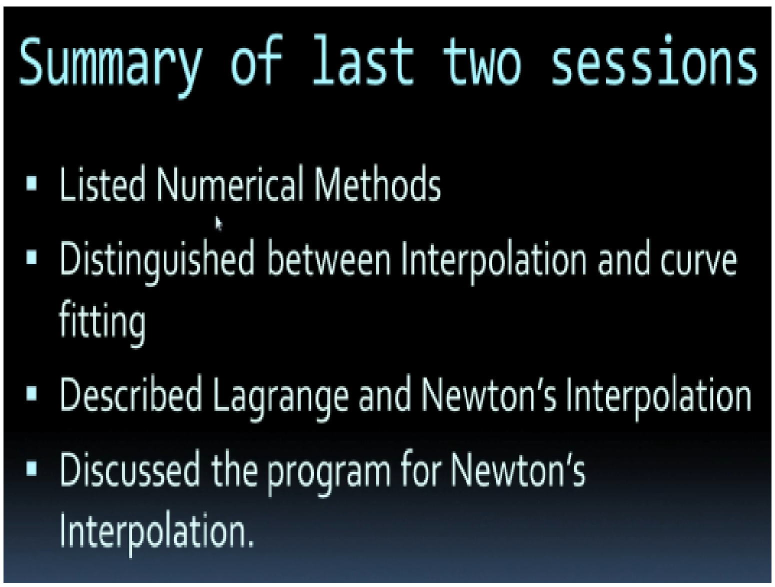

Which we want to study in this course and in particular we discussed interpolation and before we discussed interpolation, we distinguished between interpolation and curve fitting. Curve fitting also we will take up in a later lecture and in interpolation we described two methods one was Newtons method of interpolation in which we took divided differences between the values of the function and given the values of x from x0 to x n.

The functions are defined at x0 x1 x2 up to xn, so you have fx0 fx1 fxn. So, the differences between the functions are your divided differences. So, using those divided differences we interpolate. So, that was a method for Newtons interpolation then Lagrange method take the products or functions x- x1 and x- x2 xk-xn. So, these two methods we compared, we discussed the program for both the methods.

And we also said that whenever you interpolate for 4 data points using a 3 rd order polynomial, the polynomial is always unique. It is a unique interpolating polynomial whichever method you use. So, before we conclude this section, we also want to know what is the error in our interpolating polynomials. So, that is what is given here.

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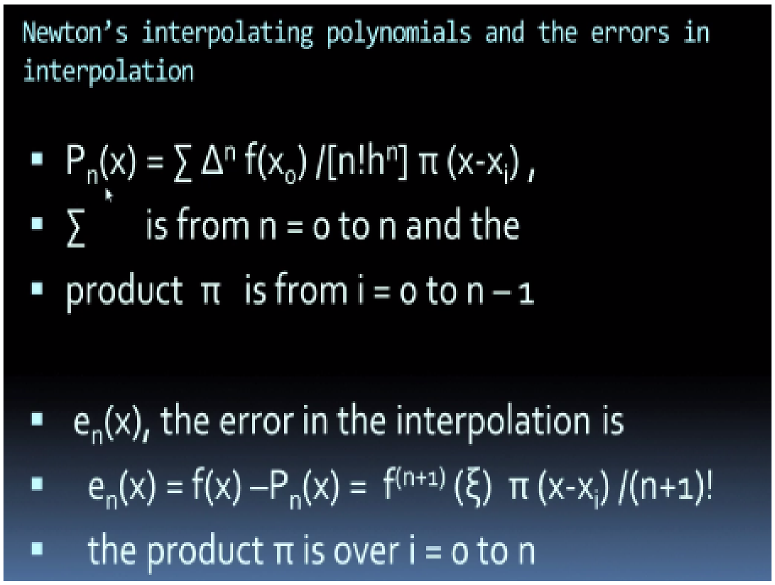

So, look at this Newtons interpolating polynomial. So, Pnx is given as sum of delta nfx0 so that is the n th order forward difference/n factorial * h to the n product of x-xi. The summation is over all the forward differences delta 1 delta 2 all the way up to delta n. So, that is my sigma going from n = 0 up to n and the product is from 0 to n-1. So, there are n-1 factors here so once I have this polynomial which is evaluated at each value of x.

I would like to know what is the error in the interpolation. So, how do I define an error the error in the nth order polynomial would be actual value of the function – the interpolated value so P nx is the interpolated value fx is the true value. Okay that difference is given in terms of tailored expansion. We will consider that at a later stage so that difference is the n+1st derivative of that function we have this function n+1st derivative at the sum value of the psi.

Okay, multiplied by all these products divided by n+1 factorial and the product is from 0 to n. That is x- x0, x- x1 all the way up to x-xn these are the products/n+1 factorial and the derivative of the function at a value of psi. This value of psi is somewhere between x0 and xn, so such analysis allows us to find out what are the errors in our method and this is very important we may not refer to it again and again.

But there are always ways of estimating the errors in our numerical methods and that is going to be important. So, we will conclude this section on interpolation now and now I shall go to the method on matrices. We will be considering matrices now that is my next task, I shall go to that. So, I will be considering all the operation on the matrices okay so now let us ask this question how do these matrices arise?

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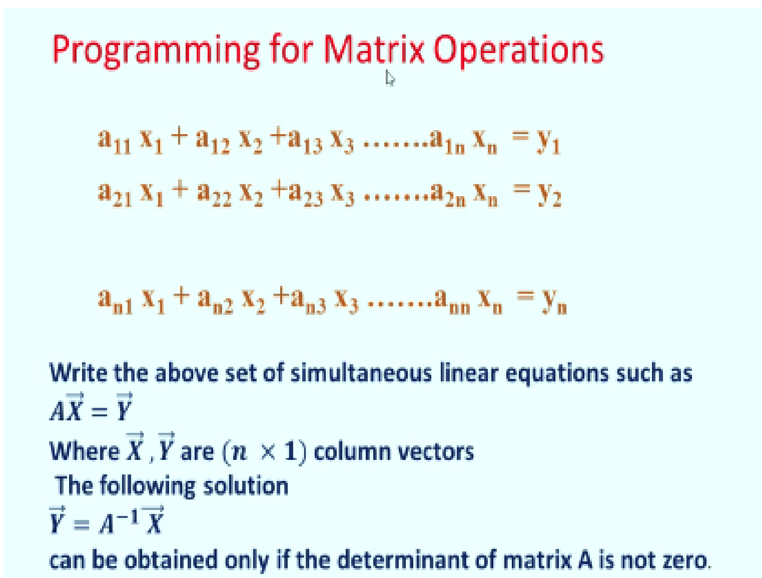

So these matrix operations arise the first time when we study linear equation, linear simultaneous equations, suppose I have variables x1 x2 x3 up to xn. I have these n variables x1 to xn and I want to get the solutions to such equations okay, so the first equation is a11 x1 a12 x2 a13 x3 up to a1n xn this is my first equation between the n values of x. So, the second equation is a21x1 a22x2 a23x3 all the way to a2nxn.

So, the first equation=y and y1, the second equation=y2, so the last equation a n1x1+an2x2+an3x3 and the last term is annxn=yn. So, I have my right side is y1 to yn and my left side they are n equations and they are n equation for n unknowns. What are my unknowns?

x1 x2 x3 up to xn. So, there are n unknowns only if n equations then I have a unique solution. For example, suppose you have a simultaneous equation for two variables x and y.

If I have variables x and y and if I have two equations for this x and y then only, I can solve it because if there is only one equation between x and y then I do not know the values of x and y independently. At best I can express x in terms of y for example ax+ by = 0. This is an equation so my ax=- by and x will be –b/a*y so I have solved x in terms of y. I have no independent answer for x.

Because I have only 1 equation between x and y a so if I have two equations between x and y I can solve it uniquely, so this is an example which is generalizes that equation for x and y * equation for x1 to xn. So, there are n equations and n unknowns and n values of this y1 to yn so one way to solve it would be represent this whole thing as matrix equation. So, what is the matrix equation?

My right side y I write it as a column vector y1 y2y I write it as a column vector That is my y left side is a column vector x. So, what is this column vector x1 x2 x3 x4 up to xn and this is my column vector x. Now A is a matrix which multiplies a column vector X and gets a product Y, so AX gives me Y. Okay what is A now this is n/n matrix. These are my values for that n/n matrix a11a12a1n.

And it is my first row and this my second row, and this is my n row. So, this is n/n matrix so when I solve this equation AX=Y. I can get a solution provided I get an inverse of the matrix okay I shall define an inverse shortly. All I have done A*X=Y so suppose on the left side I multiple by A inverse A inverse*A is 1. So, X will be A inverse Y okay, so this is how I write the solution for this.

Okay to solve for this equation I need to find out what is A inverse okay so actually this should be X inverse sorry X should be A inverse Y. This is the mistake here it is not Y is not equal to A inverse X actually Y=AX you see that Y= AX so if I want X I should take A inverse on the left side A inverse*A will be A inverse*Y so please read this as A inverse*Y will be X and I am solving for X.

So, what is the main requirement here I need to get A inverse and to find A inverse I need to have a determinant. Because only if I have a non 0 value of the determinant then I can get A inverse so that is what is shown in the next line so let us go to next slide.

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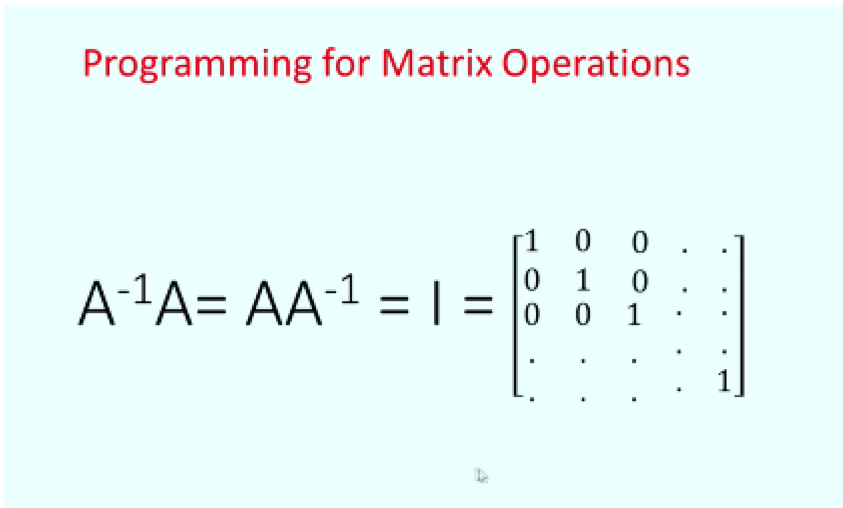

Before I go to this let us define A inverse now A was already define in the last slide what was A? It is n/n matrix A11 A12 A1 N. This is my first row A21 up to A2N is the second row, so I have this matrix A if I can get it inverse and the product of this is my identity matrix. What is an identity matrix? All the diagonal values are = 1 and all of diagonal values are equal to 0. This is my identity matrix and what is the property of an identity matrix.

Multiple any matrix by identity matrix, I get the original matrix and the other thing, so this particular multiplication A inverse*A gives me I and also even A*A inverse also gives me I. So, whether I multiple A inverse on the left of A or on the right of A I get the same result. This is true only for this multiplication. And in general matrix multiplication is not commutative. What is the meaning of that?

AB the product of 2 matrices A and B is not equal to B*A. So, verify this taking any two simple 2/2 matrices. Take 2/2 matrices and in general they will not commute that is the product depends on the order of multiplication. But if one of the matrices is I then there is no problem because the identity matrices commutes with all the matrices. So, what is my next task my next task is to define the elements of this A inverse.

So, A inverse is the inverse of matrix A and now I want to define the elements of A inverse.

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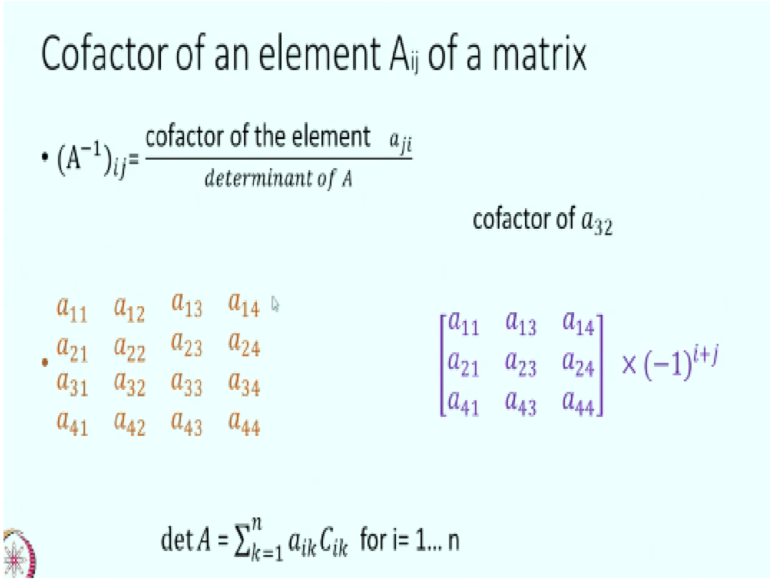

So, this is the formal definition of the inverse of this matrix so ij th element of the inverse, so A inverse is the inverse of matrix A ijth inverse is given by the co-factor of element aji divided by the determinant of A. So, to determine the ijth element I need to determine the co-factor of element aji. So, before I go to the co-factor of the element aji let me generally define what is a co-factor.

So, co-factor of a32 so what is a32 the third row and the second column of this matrix, a32 is the element which is the 3rd row, 2nd column. So, the co-factor of this particular element each element will have its co-factor which is given by the determinant of a matrix which is obtained by deleting that row and that particular row and that column. So, if I want co-factor of a32 I delete the 3rd row, I delete the 2 nd column and I get the determinant of the lower order matrix.

So, this particular matrix will be 1 order < this because A was a 4/4 matrix the determinant corresponding the co-factor will be 3/3 matrix. So, the determinant of the matrix multiplied by -1 to the i+j so what is i+ j, I was =3 and j was =2 so, I multiply -1^ i+ j. What is the meaning of that? Whenever i+j is odd there will be a - sign associated with the determinant and whenever i+j is even there will be a+ sign.

So, what will be a co-factor of a11 for a11 I delete the first row and the first column, it will be determinant formed by the remaining values 3/3 matrix starting with a22 a23 a24 all the way up to a42 a43 a44. I get the determinant of this and multiply by -1 to the i+j, i+j was 1 and 1 here so there will be a+ sign. So, whenever I get a co-factor of a11 a22 a33 a44 always the sign is going to be positive.

Because when both i and j are equal i+j is always even so the co-factor of all the diagonal elements will have a+ sign here and of course you can remove the appropriate row and column to get the co-factor. So, that is how I defined the element of my inverse matrix so when you get the ijth element of the inverse matrix. Note carefully so I need the cofactor of the element aji so if it is ijth element.

I need the co-factor of ji element and divide by determinant A so since I have defined the element of the inverse. I also need to know define the determinant, so you know that determinant of a 2/2 matrix. Let us say A B C D will be AC –BD it is known, and it is simple case it is 2/2 case it is 2 terms. So, when I have large number of rows and columns so my determinant A for a larger than 2/2 matrix will be given by this definition.

This is my definition of the determinant what is the definition? sum going from 1 to n and K is going from 1 to n aik and Cik so that is I take ith row so let us say i=3 so it will be a31*C 31 a 32*C32 a33* C33 and a34 * C34 so to expand this determinant I can expand from any row or any column. In this case I gave this example of expanding from 3 rd row instead of 3 rd row I can also expand from 1st row.

So, when I expand from 1st row a11 * co factor of a11 cofactor of a11 will be this particular matrix whose determinant I take. So, a determinant can be expanded by any row and any column, so I will get the same value of the determinant regardless of how I do. So, what have we done in this particular slide we have given the definition of the determinant and we have given the definition of the elements of the inverse matrix.

Now we go ahead outline a procedure how I get the determinant as well as inverse of the given matrix. So, before I proceed further suppose you want to find the determinant by multiplying all these quantities so for a 2/2 matrix the determinant consist of two terms for 3/3 matrix. It will have 3 factorial terms. So, for a n/n they will be n factorial terms which I want to calculate all the n factorial terms and then add them to get the determinant.

As you know n becomes large n factorial becomes very large for example try to calculate what is 13 factorial. So, I need 13 factorial terms to calculate the 13/13 determinant and my assessment is that if you want to calculate 13/13 determinant by hand calculation without using the computer you think this method using this method, even your whole life time may not be sufficient to convince yourself that this is right.

Calculate the time you will require to calculate say a 6/6 determinant by hand okay so now I shall go to the next slide which gives me the procedure to obtain this inverse of this matrix so what procedure I am going to use. The procedure I am going to use is that.

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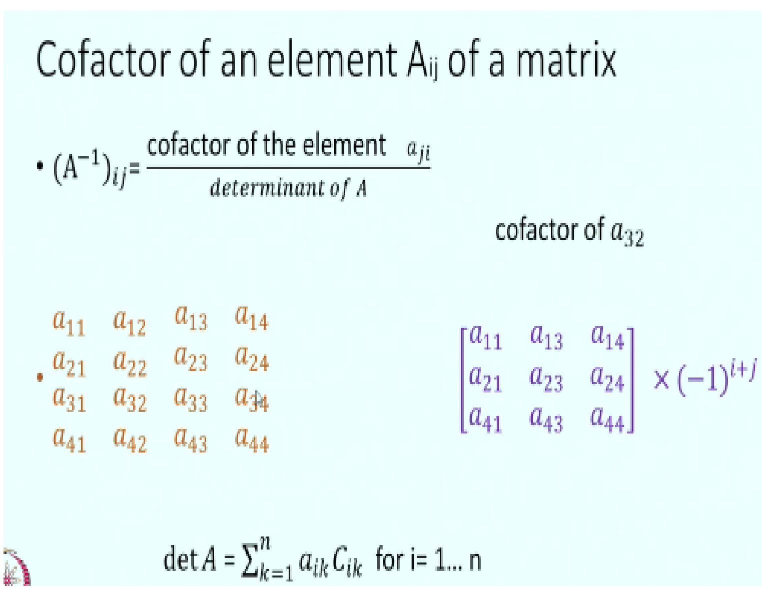

Once I have matrix like A, I will convert this matrix by multiplying several matrices on the left so that the diagonal elements are converted to 1 and of diagonal elements are converted to 0. So, I am going to multiple by various matrices on to this matrix A from the left side and convert this matrix in to an identity matrix and let us see what are those 3 particular operations.

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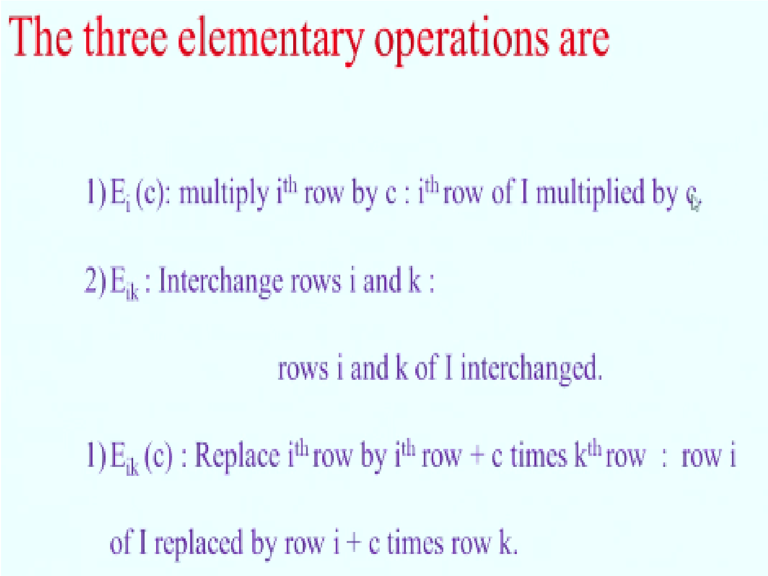

These are called elementary operations. They are three elementary operations we will illustrate with examples for all these three operations. So, first operation in Eic so what does this operation do. It multiplies the ith row of any matrix by constant c, so I want to multiple the i th row of any matrix by constant c. How will I do that I take an identity matrix and the ith row and ith column of this identity matrix is multiplied by c, so it is a diagonal value identity matrix.

It has only diagonal values, so if I take the diagonal value of the i th row and ith column in to c of the identity matrix and multiply a given matrix by Eic. I will have a situation where the ith row of this given matrix is multiplied by c. So, that we will take in the example in the next slide, so this is my first elementary operation What does it do? It multiplies the ith row of the given matrix by constant c.

The second elementary operation is suppose I want to exchange rows i and k of a given matrix I want to exchange i and row so to exchange i and row. I go to the identity matrix exchange i and k of this identity matrix and then multiply by this exchanged identity matrix onto my original matrix So, this is my second operation exchanging elements of a given matrix, so the third operation is called Eikc.

What is this third operation replace the ith row of a given matrix, by ith row+c times kth row remember I have i th row and I take k times sorry c times kth row. So, when I do that what will happen to my original matrix? I have row i of the original matrix which is replaced by row i+c times row k. So, to do that I take that identity matrix okay replace the identity matrix itself by i times the c times row k is added to row i. I will give you the examples.

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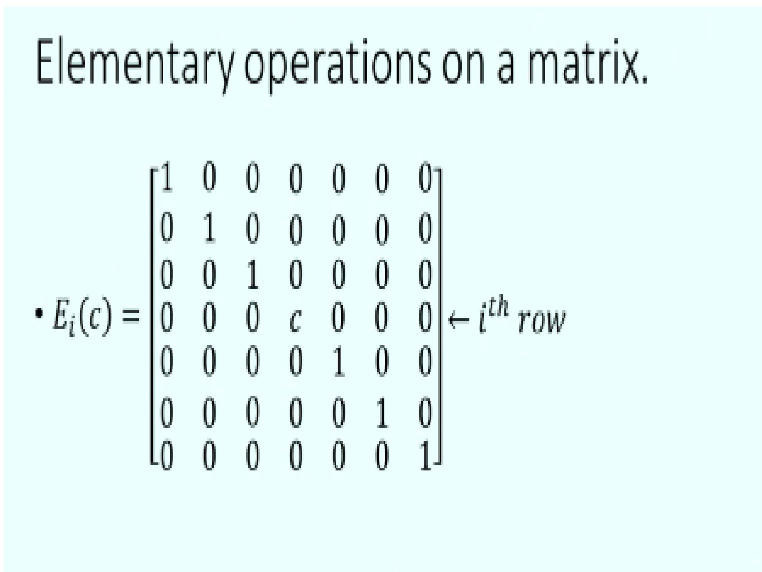

So, let us now consider that example here. What is Eic? So I have the identity matrix the ith row of the identity matrix is multiplied by c, so all these other elements are 0. So, only the diagonal element of matrix c is multiplied. Diagonal element of this matrix is replaced by c in place of one. So, if I take this matrix and multiply to a given matrix verify yourself that you will get c times the original matrix.

So, that is shown here that you verify yourselves and the question I will ask you is instead of trying to convert the c th row of a matrix by c times that row. Suppose I want to change the cth column of that Matrix. Suppose I have a matrix a and the entire column of that matrix I want to multiply by c times that particular column. Just think about how you go about getting this particular result.

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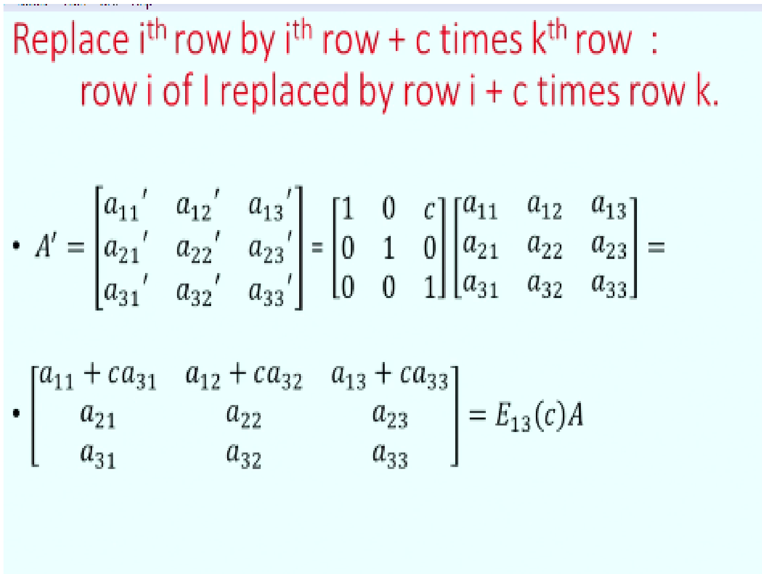

So, what I will show on the next slide now, so this is my What have I done here? I have taken the identity matrix in that identity matrix I have multiplied c times the 3rd row This is my 3rd row of the identity matrix. Suppose for this, I multiply by c, so I will have 0 0 c so that I have added to the 1st row that is c times the third row is added to the 1st row for the identity matrix. So, with such a matrix I am multiplying my original matrix a11a12a13.

So, what will happen when I multiply this is my result, what is my matrix multiplication, the first term will be the 1st row of this matrix, multiplying the first column of this matrix. So, what is that 1*a11+0*a21+c*a31 so that is my first value of the product that is what is written here a11+ c times a31 so that is the first row and the first column. What is the second row and column 1* a12 that is what is given here.

That is a12+0*a22 which is 0+ c*a32 so a12 * c times a32 what is the 3rd element 1*a13+0*a23+c*a33. So, that 1st row of this particular product now is a11+c times a31+a12+ c times a32+a13+c times a33. All the other two elements will remain unchanged because see the 2nd one now when I multiply this particular 010 to this 2nd particular column, what we will have 0+a21+a31.

So, my second row and first column of this second of these matrix A prime is a21 similarly the next one will be a22 and next one will be a33 a23, so the second row remains unchanged. The third row remains unchanged so what I have done by this called the elementary matrix, they are three elementary matrices. So, this is the most difficult one I have shown you that if I multiply E 13 times c and multiply on the left side of a what I get is the first row of a.

Change to its original first row+c times the 3rd row that is a13 E of 13 of c into a. So this is how I can manipulate my original matrix and get my results of choice. So, now let me summarize this gauss algorithm so before I summarize, I think I should take one example. Okay, I think it is all right I shall just summarize my algorithm because we will have to use this algorithm throughout our program.

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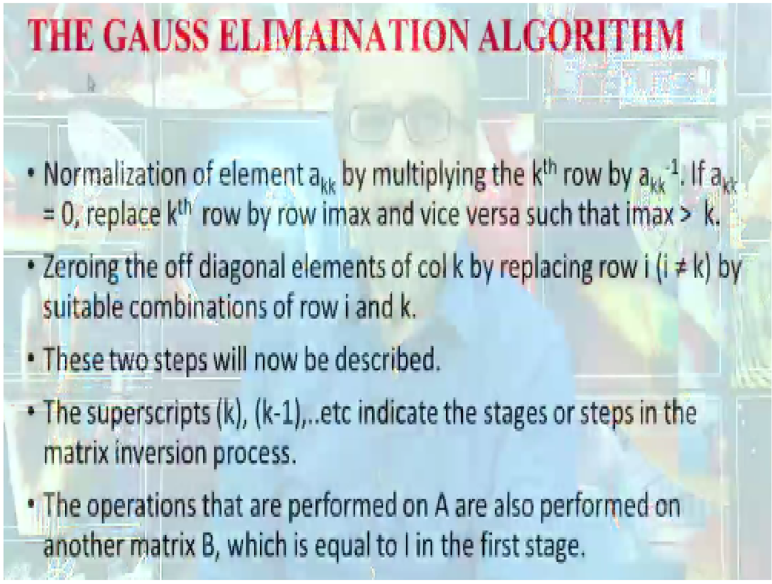

So, what is my gauss elimination algorithm? Whenever I have a matrix suppose I have element a kk so what I want to do I want to normalize that element akk by multiplying the kth row by 1/ akk so what will happen when I multiply the Kth row by 1/akk the diagonal element will become 1 that is normalization and it may so happen that akk is 0 so if a kk is 0 I cannot divide by 0. So, what I do in that case.

I exchange k th row by some other row such that I replace my k th row by another row who has the maximum element in that particular row. So, such that Imax actually of course greater than k so I exchanged two rows if that akk is 0 so first part is normalizing that particular row kth row then the second will be the off diagonal elements of column k.

So, the diagonal element I have made it 1 and all the non-diagonal elements off diagonal elements, I convert them into 0 by replacing the ith row by combination of row i and k. So, I take combination of row i and k to 0 off the diagonal elements. So, now these 2 steps I shall describe so what will I do now in my remaining slides, the super scripts k k-1 etc will indicate the stages or steps in the inversion process.

And whatever operations I do on matrix A, I shall also perform those operations on matrix B and what is my matrix B is equal to identity matrix in the first stage and the remaining stages it will go on, including all the results of operations which are done on the left side. So, now let us take an example how to use this Gauss elimination algorithm.

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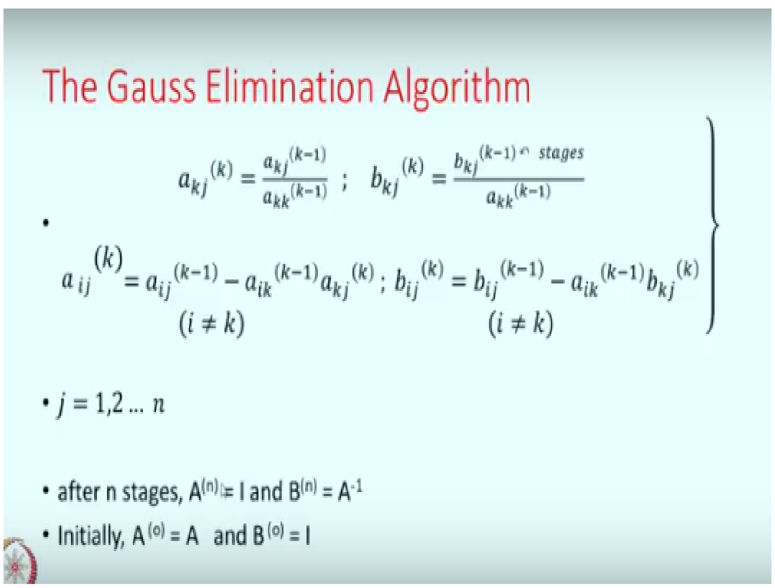

So, this is my Gauss elimination algorithm, whatever I said in words is given here. I shall come back to this algorithm after I take an example so let me take an example and come back to this procedure.

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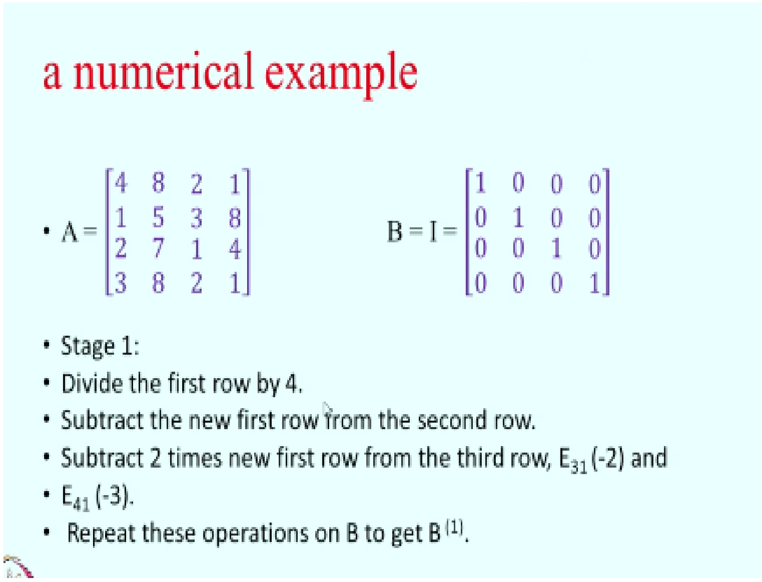

So, in my numerical example okay, what I have done is I have taken a matrix A, matrix A in these case is 4 8 2 1, second row is 1 5 3 8 and the third row is 2 7 1 4 and the last row 3 8 2 1. My matrix B is an identity matrix This is my starting point for matrix B this is my original matrix so now I want to do all the operations on matrix A and B so that I get a identity matrix So what is the first task?

The first task will be either divide the first row by 4 so this is my 1st row I shall divide every element of this row by 4. So, what will I get? 4/4 is 1 8/4 is 2 2/4 is 1/2 and 1/4 is 1/4th. The same thing I will do for this so when I divide this by 4, I will get 1/4 0 0 0. So, first I shall convert the diagonal elements into 1 and all the off diagonal elements in to 0. Then the next time I want to 0 these off the diagonal elements 1 2 and 3.

How will I do that? I take the new 1 st row and take suitable combinations of these new 1 st row and add it to the 2nd row and how will I do that? I will do all this by elementary operations so what we will do, we will conclude this lecture now. In the second lecture I shall again begin at the same point and convert the matrix A in to its diagonal form. So, I shall conclude the present lecture here and in the next one I shall continue exactly where I left at this point. Thank you.