Computational Chemistry & Classical Molecular Dynamics
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Lecture – 17
Gauss Elimination Method for Matrix Inversion

Hello and welcome to this lecture which is a continuation of the lecture on inverting the Matrix by Gauss Elimination Method. What we do in this elimination method is that I have a matrix A and I convert all the diagonal elements of this matrix into identity matrix and set all the off diagonal elements into 0 by multiplying the given matrix by three elementary operations. So, what are these 3 elementary operations?

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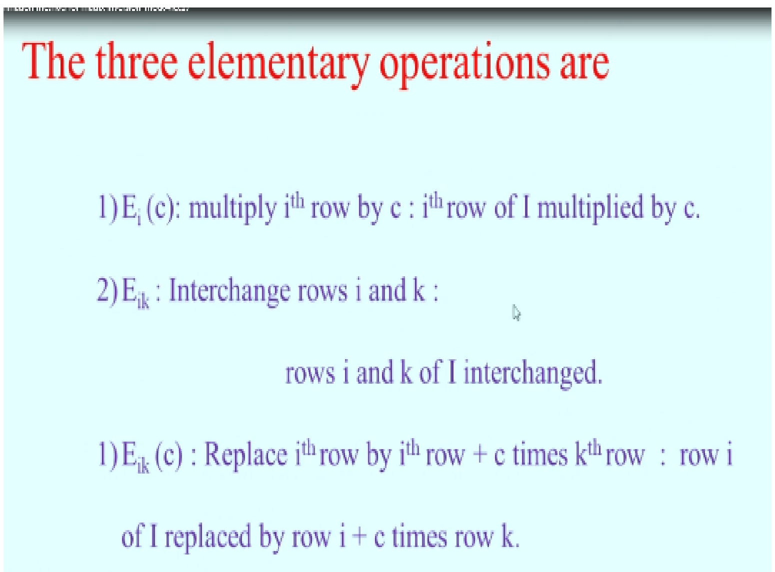

The first operation is multiplying the ith row of a given matrix by a constant c how do I multiply given matrix and get its ith row multiplied by c. I take this identity matrix in that identity matrix I multiply the ith row by c. So, that is very easy to do just convert the diagonal elements in the ith row by c and multiply the original matrix what is the next one? Exchanging rows i and k is I take the identity matrix and exchange it ith and kth rows that is very easy to do.

Ith row have diagonal Ith row had diagonal 1 here in kth row the kth diagonal was 1 when you exchange in this new matrix the two diagonals in i and k will not be 1 because you have exchanged them so that is my Eik exchange. I exchanges rows of the identity matrix ith row and kth row what is Eikc? ith row replace the ith row by c replace the ith row by c times the kth row so examples are given in the next slide see this is Eic,

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Elementary operations on a matrix.

- $E_i(c) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \leftarrow i^{th}\ row$

What is Eic? The cth ith row and the ithcolumn is such that one is multiplied by c, so this is c times the ith row. This is my Eic so what is Eik? Eik would be ith row and kth row exchange suppose kth row was this particular row. 1 2 3 4 5 6 if 6th row is the kth row and 4th row is the ith row When I exchange them the 4th row the new 4th row there will be k in the 6th row and there will be 1 in the 6th row here and 1 in the 6 th row.

There will be 1 in the 4th column and in the 4th row there will be 1 in the 6th column because i have exchanged the 4th row and the 6th row that is my exchange value and the 3rd one is.

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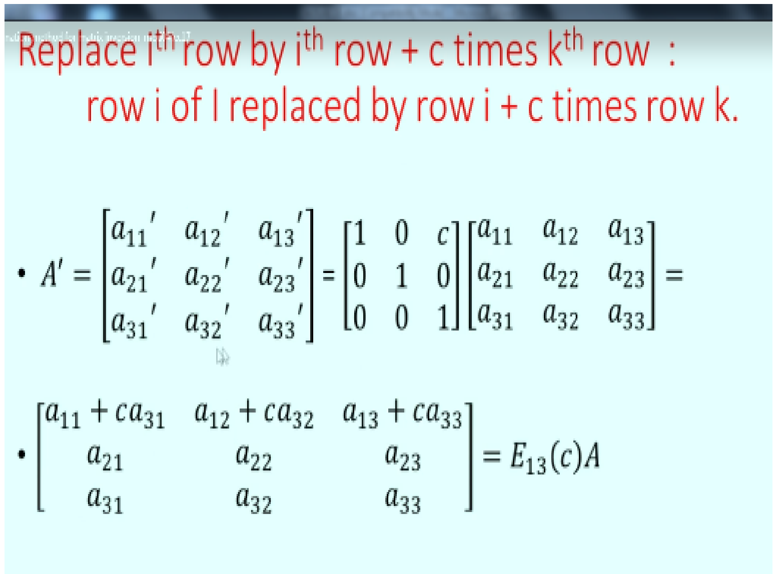

Eikfc so this is E13 of c what is that? My 1st row is replaced by original 1st row but what is my original 1st row 1 0 0 I have replaced it by original row + c times the 3rd row c times the 3rd row what is c times the 3rd row? 0 0 c so when I add 0 0 c to 1 0 0. I get 1 0 c so this is that E13 of c so what is the effect of E13 of c multiplied onto the original matrix? What I get the new result is the original row + c times the 3rd row.

So, if an original row + c times the 3rd row I multiply on the left by E13fc, so this is my method. so before I give a numerical example, I will give this algorithm.

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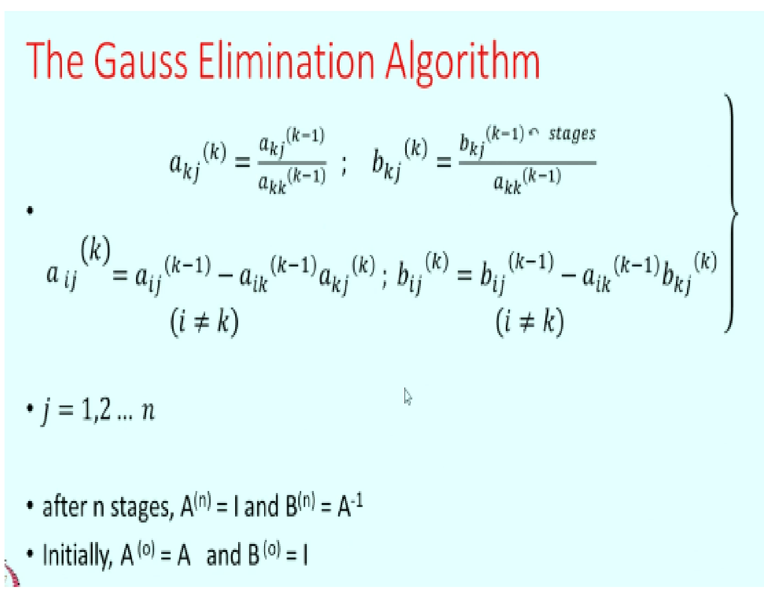

Which is called the Gauss Elimination Algorithm what are we doing in the Gauss Elimination Algorithm the kth element the kth row is multiplied by akk so what are these super script k and k-1 these are the stages so if I want to go from k – 1st stage to the kth stage I take the old matrix in the k- 1st stage in our case let us say if k=1 this is just the original akj divided by akk, so I am taking the kth row and dividing the kth row by the diagonal elements of the kth row.

So what will it do? It will convert the diagonal elements into 1 and whatever I do to my matrix a the same thing I do to matrix b what was matrix b? It was an identity matrix to begin with so in the kth stage I take the k- 1st stage bkj and divided by ak k -1. So whatever I am doing to matrix a, I shall also do to matrix b, so I will get the kth stage of matrix b from the k- 1st stage. this is for my kth row.

Then what do I do 2 rows other than k? Suppose now I want i0= k for the remaining rows so I take now I want the value for the remaining rows. What do I do that I take the old row this my old row k-1 is the old I want the new value now old row- aik of the old row multiplied by akj of the new row so the new matrix is a k j of this is my new matrix or the new row, so the new row multiplied by ai k-1 as the previous version previous stage.

Then when I do that it will convert all the non-diagonal elements into 0 so this will show by an example so when I do this all the non-diagonal elements will go to 0 and whatever I do to matrix a I shall do exactly to make this b so this I shall do for all the other j. So now how many stages will be there? There will be n stages now after the n stages the matrix a in the n stage will become identity matrix and the matrix b will become the A inverse.

So what is the initial condition? Initially a 0=a and b 0=i so I do n stages what is this n= number of rows or columns after this n stages I will get the original matrix become the identity matrix and the original identity matrix become the A inverse so this is my gauss algorithm. It is also called Gauss Jordan elimination method.

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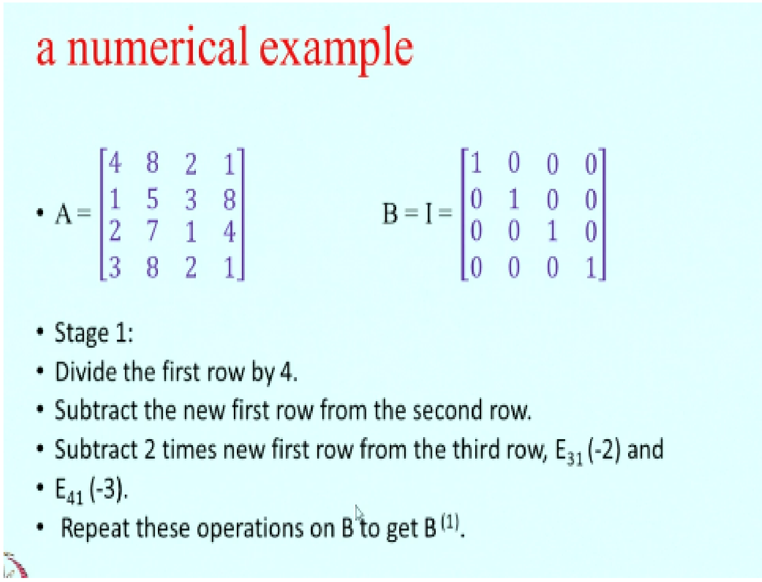

So, now I will take a numerical example so my numerical example I had illustrated this little bit in the last lecture, so my matrix is 4 8 2 1 this is my 1st row 1 5 3 8 2nd row, 2 7 1 4 3rd row and 3,8,2,1 is my 4th row and what is my matrix b? b is the identity matrix 1 1 1 1 the rest are all 0. So what is my strategy now? The 1st row I had this 1st row I will convert the 1st value 4 to 1 and the remaining these 3 values, I will convert them to 0.

How will I convert this 4 * 1 by dividing the entire row by 4, so that is my first operations divide the 1st row by 4 so how will I do that? I will do that identity matrix and the 1st row and 1st column of Identity Matrix will be 1/4 because when I multiply by 1/4*4 I will get 1 so that is my first operation. What will I do in the second case? so in my new 1st row will be 1 2 1/2 1/4 because I have divided this by 4.

So, new value of this is 1 now so if I subtract the new 1st row from the 2nd row if I just subtract, I will get 0 here so that is what I am doing here subtract the new 1st row from the 2nd row. What was the new 1st row 1 2 1/2 /1/4? so I subtract from the 1st row this will become 0 now subtract 2 times the new 1st row from the 3rd row because 3rd row this element is 2 so only when I subtract 2 from this 2, I will get 0.

So, my new row was 1 so I subtract 2 times the new 1st row from the 3rd row so what do I do for the 3rd row now? I subtract 3 times the 1st row new 1st row from here so 3-3 will be 0 so that is what I do so what are my operations now? If I want to subtract 2 times the 1st row from the 3rd row it is E31- 2 because -2 means and - 2 times the 1st row, I am adding to the 3rd row so what is the last 1? so - 3 times the 1st row is added to the 4th row.

So, that E41-3 so when I do these operations you will see the result in the next slide but exactly the same things, I will do on the matrix B which was i begin with so let us see the next slide.

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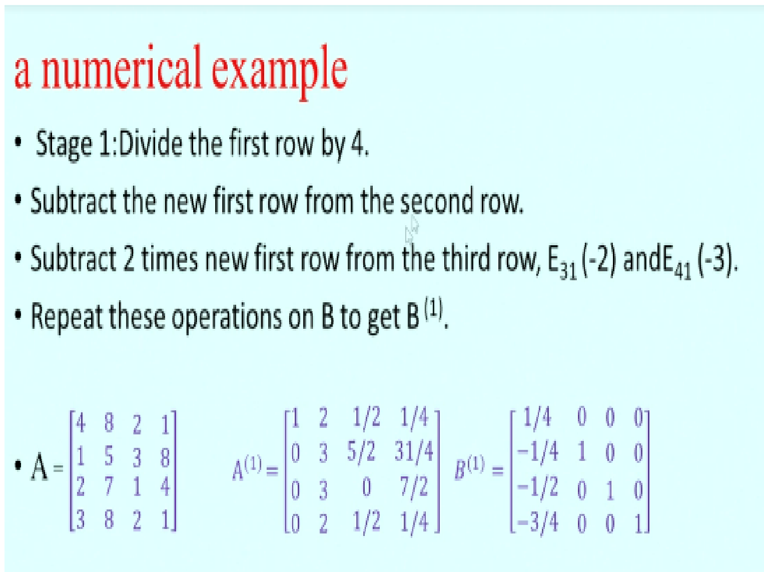

So what was the numerical example?1st Stage 1 divide the 1st row by 4 look at this and repeating what I said earlier because it is only when you do an algorithm by hand you will understand the algorithm very clearly because only when the computer does everything for you do not see all the operations and if the operations are not correct you will get an incorrect result and it takes quite a bit to understand what went wrong in your computer program.

So, if you know a numerical method and apply the computer program for this numerical method every step will be cleared so the 1st row has become 1 2 1/21/4 what I have done in the next stage subtracted this new 1st row from the 2nd row what do I get? 1-1 is 0 5-2 will be 3 then 3-1/2. Because I am subtracting from the old 2nd row I am subtracting the new 1st row so 3- 1/2 will be 5 1/2 and – 1/4th will be 31/4.

So, from the 2nd row I have subtracted the new 1st row what will I do for the 3rd row? I subtract 2 times the 1st row so 2–2 times 1 is 0 7 - 2 times 1/2 I have 7 here. I need to subtract 2 times 1/2 so that is 1 so actually this is not correct this should have been 6. Now what is the 4th row? This is the last element I multiply 2 times this what is 2 times 1/4? 2 times 1/4 is 1/2. So, I am subtracting 1/2 from 4 I will get 7/2.

So, this 0 is incorrect, so correct it appropriately how do I correct it? 7-2 into this that is 1 so it should be 6 so correct this 0*6 and what is my last row now? 3-3 times 1 that is 0 then 8–3 times 2 3 times 2 is 6 so 8–2 is 2. So, I have 2 here then 2-3 times 1/2 3 times 1/2 is 3/2. When I subtract 3/2 from 2, I will get 1/2 and what is my last particular element? 1-3 times 1/4th is 3/4 when I subtract 3/4 from 1.

I will get 1/4 so this is my new A what is the a obtained after the 1st stage? In the 1st stage I have made the diagonal value of the first row into 1 and all the off diagonal elements to 0. So, my 1st stage will be these 4 operations these 4 operations are 4 elementary matrices. I did all these 4 operations by multiplying by A4 elementary operations on the left side. So that is my end of stage 1.

So, similarly for stage 1 of B so B1 will be exactly the same operation that I did on a I will do on B so as a result what will happen? The 1st will be 1/4 because I have divided the 1st time by 4there is 1/4 and all the remaining I have obtained from whatever operations I did on matrix A and matrix B, so you see that as the 1st row 1st column of my original matrix is replaced by 1 0 0 0. The 1st column of my matrix B is replaced by other objects.

All the other elements of B are unchanged so what will be my strategy for the 2nd matrix now for the 2nd stage so I shall start with a diagonal element of this, so I shall divide the 2nd row by 3 so which is the 2nd row now second row on a matrix of the last value obtained in the stage 1. A1 is the last result of stage one so I will make this 3 into 1.

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$$A^{(1)} = \begin{bmatrix} 1 & 2 & 1/2 & 1/4 \\ 0 & 3 & 5/2 & 31/4 \\ 0 & 3 & 0 & 7/2 \\ 0 & 2 & 1/2 & 1/4 \end{bmatrix} \qquad B^{(1)} = \begin{bmatrix} 1/4 & 0 & 0 & 0 \\ -1/4 & 1 & 0 & 0 \\ -1/2 & 0 & 1 & 0 \\ -3/4 & 0 & 0 & 1 \end{bmatrix}$$

Stage 2:

a) Divide the second row by 3, E_2 (1/3).

b) Subtract two times the new second row from first row. E_{12} (-2)

c) E_{32} (-3).

d) E_{42} (-2).

$$A^{(2)} = \begin{bmatrix} 1 & 0 & -7/6 & -59/12 \\ 0 & 1 & 5/6 & 31/12 \\ 0 & 0 & -15/6 & -17/4 \\ 0 & 0 & -7/6 & -15/12 \end{bmatrix} \quad B^{(2)} = \begin{bmatrix} 5/12 & -2/3 & 0 & 0 \\ -1/12 & 1/3 & 0 & 0 \\ -3/12 & -1 & 1 & 0 \\ -7/12 & -2/3 & 0 & 1 \end{bmatrix}$$

So, that is my next slide let us look at this so what do I do? This is my A1 and this is my B1 exactly the same results that I had from the earlier slide so what will I do? Divide the 2nd row by 3 so how do I do that? Take the identity matrix it E and the 2nd row of this identity matrix is replaced by 1/3 instead of 1 so I am going to divide the 2nd row by 3 so I will take this E2 1/3 so E2 1/3 is the identity matrix where the 2nd row is replaced by 1/3 so what will I get?

0/3 is 0 3/3 is 1 5/2 divided by 3 will be 5/6 and 31 /4 divided by 3 will be 31/ 12 see this is what has happened in A2 so the 2nd row of A2 now 2nd row of A2 is the original row divided by 3. That is my operation so my 2nd row is 0 1 5 /6 31/12 so similarly the second row of B2 will also change let us not worry about B2 right now so once I have this as my 2nd row what do I do now? now I have to make sure that the 2nd row of A1.

Entire 2nd column of A1 the diagonal element has already become 1 now the off diagonal elements I want to make it 0 so how do I make the off diagonal elements 0? So, this is my 2nd row here so to make the off diagonal elements 0 I subtract 2 times the 2nd row from the 1st row here. What will happen? 2 times 1 will be 2 so when I subtract 2 from 2 i get 0. So, I want to make the entire 2nd column other than the diagonal element to be 0.

So, to convert this 2 * 0 I take the row after the 1st stage and the 2nd one I take this row multiplied by 2 times this and I subtract from the 1st row so that is my statement here subtract 2 times the new 2nd row, this is my new 2nd row subtract 2 times this from my 1st row here when I subtract that what I will get is 1 0 -7/6 -59/12 so let us see how I got this -7/6 what did I do 2 times 5/6 will be 10/6 I subtract 10/6 from 1/2.

What is 1/2is nothing but 3/6 when I subtract 10/6 from 3/6, I will get -7/6 similarly I have 31/12 here now I take 2 times 31/12 that is 31/6, okay when I subtract 31/6 from 1/4, I will get -59/12 do that operation to convince yourself that the new 1st row in the 2nd stage new 1st row will be 59/12 similarly what do we do I have 3 in the 3rd row here so I want to set this 3 to 0 so how do I do that?

This is my old 2nd row multiply this by 3 so when I subtract 3 times the 2nd row from the 3rd row that what is near E32(-3) that is take 3 times the 3rd row and subtracted from the 2nd row so this is what it is. So this 3 becomes 0 and have to subtract 3 times 5/6 what is 3 times 5/6? That is 5/2 so I have to subtract 5/2 from this 0 so when I subtract 3 times 5/2 from this 0, I should get check this so let us see the last one.

I have 31/12 3 times 31/12 is 31/4 so I am subtracting 31/4 from 7/2 7/2 is same as 14/4 so 14-31 is 71, sorry 17 I get 17/4 similarly I take 2 times this particular row and subtract it from the last row of A1 so when I do that, I get 0 0 -7/6 -15/2 so this is my matrix that results from at the end of stage 2. What the stage 2 involved, 4 steps dividing the 1st row by 3, subtracting 2 times the new 2nd row from the 1st row so all these 4 operations are all the operations on stage 2.

So, how did I execute I multiplied my original matrix A by these 4 matrices on the left side so 1st stage also we have 4 steps 2nd stage also we had 4 steps so at the result of my 2nd stage my A2 has become this matrix and B2 has become this so what are the main observations here you will see that the diagonal element of the A2 has become 1 2nd stage and all the off diagonals have become 0 and on my matrix B both the 1stand 2nd columns have changed.

And the 3rd and 4th columns have not changed at all.

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$$A^{(2)} = \begin{bmatrix} 1 & 0 & -7/6 & -59/12 \\ 0 & 1 & 5/6 & 31/12 \\ 0 & 0 & -15/6 & -17/4 \\ 0 & 0 & -7/6 & -15/12 \end{bmatrix} \quad B^{(2)} = \begin{bmatrix} 5/12 & -2/3 & 0 & 0 \\ -1/12 & 1/3 & 0 & 0 \\ -3/12 & -1 & 1 & 0 \\ -7/12 & -2/3 & 0 & 1 \end{bmatrix}$$

Stage 3: $E_3(-6/15)$ $E_{13}(7/6)$ $E_{23}(-6/5)$ $E_{43}(7/6)$

$$A^{(3)} = E_{43}\left(\frac{7}{6}\right) E_{23}\left(\frac{-6}{5}\right) E_{13}\left(\frac{7}{6}\right) E_3\left(\frac{-6}{15}\right) A^{(2)}$$

$$A^{(3)} = \begin{bmatrix} 1 & 0 & 0 & -44/15 \\ 0 & 1 & 0 & 7/6 \\ 0 & 0 & 1 & 17/10 \\ 0 & 0 & 0 & -44/15 \end{bmatrix} \qquad B^{(3)} = \begin{bmatrix} 8/15 & 3/15 & -7/15 & 0 \\ -1/6 & 0 & 1/3 & 0 \\ 1/10 & 6/15 & -6/15 & 0 \\ -7/15 & -1/5 & -7/15 & 1 \end{bmatrix}$$

Now I have to go to the next stage what is the next stage I start A2 which is the end off stage 2 B2 which is the end of stage 2 now I want to operate on the particular 3rd column now what is my 3rd column 3rd column 3rd row this is -15/6 so how do I convert this -15/6 into 1 I have to multiply by -6/15 so this is stage 3. The 3rd row of my matrix is multiplied by -6/5. What is the result? This diagonal elements become 1 and the last element I multiply 17/4 by 6/15.

So, what I will get is -17/10 so how do I get -17/10 I have taken -17/4*-6/15 so I shall get 17/10 so that is the 3rd row which is the 1st stage of this which is the 1st step in the 3rd stage so what do I do once I convert this diagonal element into 1 now I have to convert all the off diagonal into 0 so how do I do that so this has become 1 so I want to convert this 7/6 into 0 so what do I do E13*7/6.

When I do E13 7/6 this element has become 0 and the others have changed like this. Then what do I do for the 2nd row I want to convert this 5/6 into 0 so what do I do I take 5/6 of the 3rd row with a – sign and since this is 5/6 and I multiple this by 6/5 with a – sign so when I add this becomes 0 so what do I do for the last particular column here I had -7/6 so I multiplied this by 7/6 and add.

So, when I add that -7/6 +7/6 gives me 0 and the last row last column has changed so what has happened after that at the end of stage 3 so I had A2 which is the end of stage 2*multiply e3-6/15 this is the 1st one I operated 2nd time I did E13 7/6 then E23 -6/5 and E43(7/6) I multiply by these 4 matrices on the left of A2 to get A superscript 3 so this is the end of stage 3. End of stage 3 involves again 4 steps operating on the end of stage 2 so this is my matrix.

At the end of stage3 similarly B3 has changed in this particular manner so what is remaining now only the last particular stage what is my last stage? I start with A3 which has -44/5 44/15 in the last diagonal element so I have to convert this into 1 and I have to convert all the remaining to 0 so that is my next stage.

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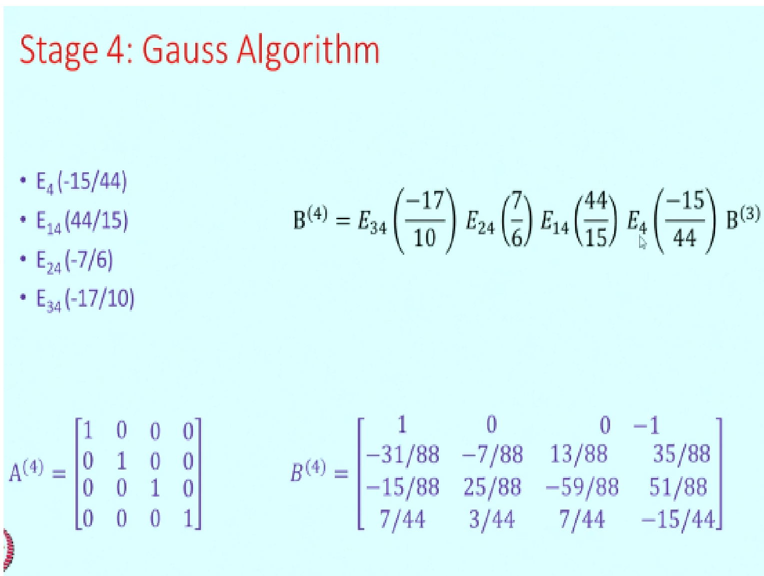

So, what do I do for the next stage? I took the E4*-15/4that converts the last diagonal element into 1 then what is the next one E14*40/15 E24 -7/6 E34 -17/10 I multiple this sequentially on A3 so I have shown here how do I get B4 now same as what I do for A3 I take B3 and on the left of B3 multiply 1st by E4 -15/44this is my 1st one 2nd 1 is E14 44/15 E24 7/6 and E34 -17/10. So, when I do this is the final result for my B4 and this is my final result for A4.

So, what has happened in this process the end of stage 4the matrix A become diagonal matrix and the matrix B become this particular matrix so what is the meaning of that? How many operations had on this original matrix? For each column had 4 matrices so when I get the last result of A4 I have multiplied on the left of the original A/16 elementary matrices. Because in each stage I am multiplying the earlier stage by 4 elementary matrices.

So, after multiplying by these 16 matrices on the left my A became diagonal and what happened to B becomes this matrix so B4 is nothing but A inverse so that is what will be on next slide let us see this again when I multiplied by those 16 matrices on the left of A I got this matrix which means that if I * by the same 16 matrices on the identity matrix what I get is my A inverse because I know that A* A inverse is identity matrix.

So, to get this identity matrix I have to multiple on the left by A inverse so that is nothing but B4 is nothing but A inverse then the other thing we wanted to do was to get the determinant, so you will find that I had multiplied by several elementary matrices and you can easily verify that the determinant of those elementary matrices is 1 except when you divide or multiply a given row.

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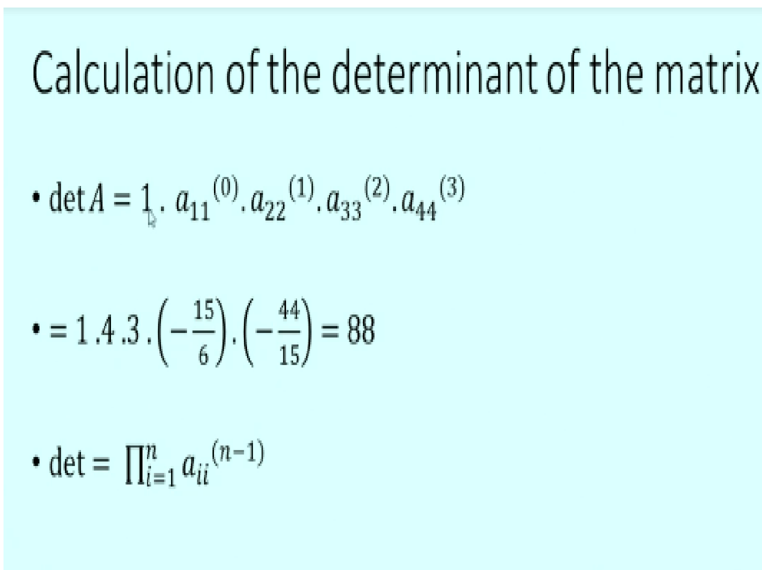

So, the determinant is given by original value a11 0 a22 1 a33 2 a44 3 what was a11 0 a11 0 was 1 a11 0 was 4 a22 1 was 3 a33 2 was -15/6 and a44 3 was -44/5 so when you multiple by all these things you get the determinant of the matrix so what is the determinant of the matrix? Product of all the diagonal values of by elementary matrices so that is my determinant.

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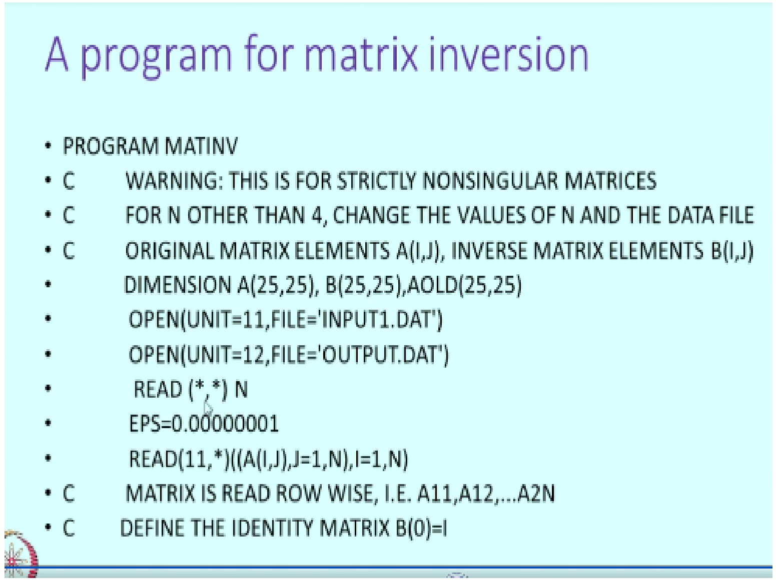

So, now what we need to do we now need to write a program to perform this elimination algorithm which is the gauss elimination algorithm, so I shall briefly describe this program I will start describing this program now we will also execute this program in our practical session so let us just see the outline of this program and then in the next class or, so I shall consider the detailed program and execute it.

So, how do we structure this program? The structure of this program would be since I am dealing with matrices, I have to deal with array variables, so I will define 3 array variables now A B C what is A now? It is a two dimensional array where each dimensional goes up to 25 so A (25, 25) means it is a 25/25 matrix. B (25, 25) means it is again 25/25 matrix. A old is an additional matrix I made need to store the additional information on A.

So, this is my dimension statement I need to declare because I am in array variables whenever I have array variables if I do not have a dimension statements, I cannot use that at all so then I need to read and write to files for that purpose I have said open (unit=11, file= input1.dat) open (unit=12, file= output.dat) and now I read n, what is n now? The particular size of my matrix if it is 4/4 my n will be 4.

So, once I read this n this, I am reading from the screen now EPS along is some variable which I shall use because many times there is no such thing as an actual 0 so we want to take in place of

0 you want to take something like 10-8 so then I shall read the entire matrix A how am I reading now? Read (11, *) (A (I, J)), (J going from 1 to N), (I going from N to 1). What is this kind of a read statement? This read statement is an implicit read statement.

So, J going from 1 to N is a do loop which takes J from 1 to N and I going from 1 to N is a do loop which takes I from 1 to N. so if N is 4 it will read 64 values of matrix A from this read statement where it is reading from? Reading from11 and that 11 is nothing but input.dat so remember that my J changes 1stand I changes later so which means I am reading the matrix row wise.

First row I read first a11, a12, a21 then 2nd row 3rd row and 4throw so it is very important when you deal with matrices to keep track of whether you are doing the row operation or column operations because both i and j are loop variables often it is confusing, so it is good to keep track of whether you are doing a row operation or a column operation. What I shall do now is I shall conclude this lecture.

I have started the program for matrix inversion, so in the next class, I shall do a little more on matrices and then go ahead with the program for matrix inversion I shall close here revise this lecture carefully because you need to know all the steps in gauss elimination method to get an inverse of this matrix, so I shall conclude here. Thank you very much.