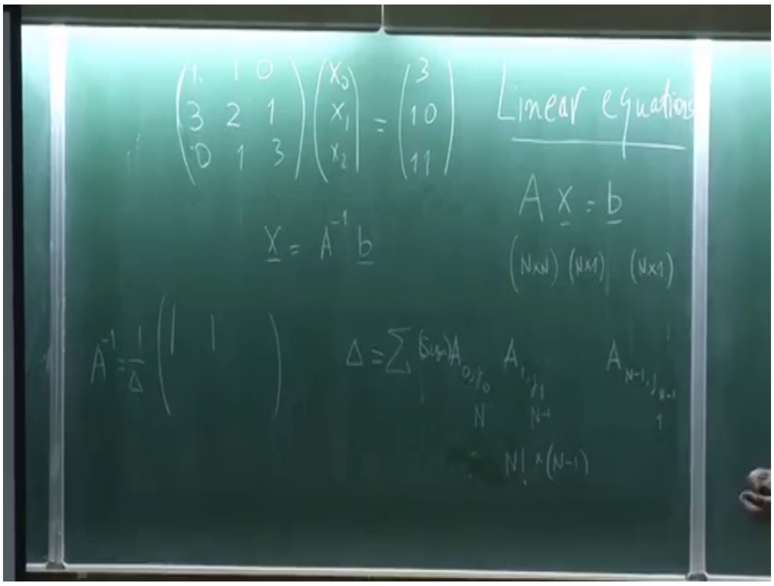
Computational Science and Engineering using Python
Prof. Mahendra K. Verma
Department of Physics
Indian Institute of Technology, Kanpur

Lecture – 26
Linear Algebra: Ax = b Solver

(Refer Slide Time: 00:15)



Linear equations.

Student: (Refer Time: 00:22).

This kept coming in the past, right when we solved a Laplacian's equation, Poisson's equation, implicit equations, right. So, there were trio-diagonal matrix which we encountered many times. So, today's class I will describe how to solve linear equations. So, we can write thing in terms of matrix; matrix A vector x which is unknown equal to b. So, this is how we will encounter these equations. Now most of the time we encounter the. So, C N by N matrix and this is N by 1 matrix and this is N by 1 matrix, right, but there are occasions when it is N by M, but that I will not discuss today at all, there are situations when encounter non square matrices.

So, let us say we have this equation A x equal to b. So, I am given b, I am given A, I have to solve for x. Now you know already in your school days, now I think matrices are taught in schools. So, x equal to A inverse b correct, but how do you find A inverse. So, A inverse involves determinants, right. So, the first; so, I mean 1 by determinant A inverse equal to 1 by determinant. Now the first entry is this matrix; sub matrix adjoint. So, it involves lot of matrices. So, for given N by N matrix, what is the complexity for computing determinant? So, I have to compute determinant right minimum, I need to do this and these are also determinants, but of N minus 1 by N minus 1 matrices.

So, how many operation do I require to compute determinant? So, first how many terms are there? So, if you know the formula. So, how do you compute determinants in terms of in computers? So, I will tell you the formula, I mean this is you have to do N loops. So, this matrix A. So, first put the first index A 0, A 1 and the last one is A N minus 1, the first the row; row index, this is row index. Now the column index will come next, but they will be all distinct, right so for determinant, when I compute the one; this, this minus this, this, right.

So, no 2; so, here all the rows are different and all the columns also must be different. So, the column I call it j 0, j 1, j N plus 1 and all the js must be distinct. Now how many js do I have? How many combinations I will have? So, N factorial because this can be any number well N minus. So, this can be yeah, this can be any number, it could be 0 as well j 0 can be 0. So, this is N options, but once I choose; this has only N minus 1 options and so on and the last one is we have no option, the Gaussian will be fix. So, number of terms, number of terms I have like these are N factorial and each of the inverse how many multiplication.

So, there are N multiplication; right with N minus 1 multiplication. So, for each of them; I have to do N minus 1 multiplication. So, I multiply by N minus 1 and then I have to do the sum. Now, sum there is a sign and the sign equal to what if all the j i's a cyclic combination then its plus if it is anticyclic combination, then it is minus. So, 0, 1, 2, 3 (Refer Time: 05:02) minus. So, this is how we computed a matrix. So, you can write a loop and you have to do product and do the sum. Now this very expensive; what is N factorial; roughly; how do we compute N factorial? So, if some function are well, I would like either exponential or power law or estimate.

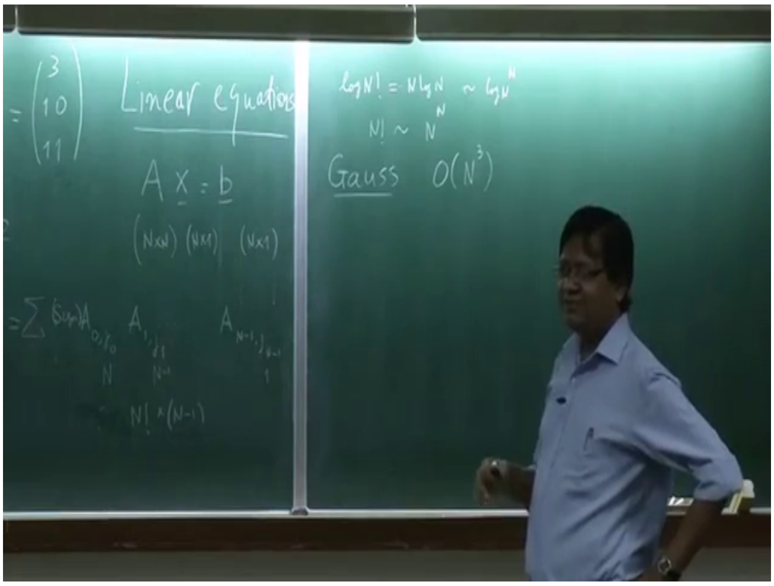
Student: (Refer Time: 05:28).

N squared, no.

Student: (Refer Time: 05:31).

So, what is sterling formula I mean these are very important.

(Refer Slide Time: 05:35)

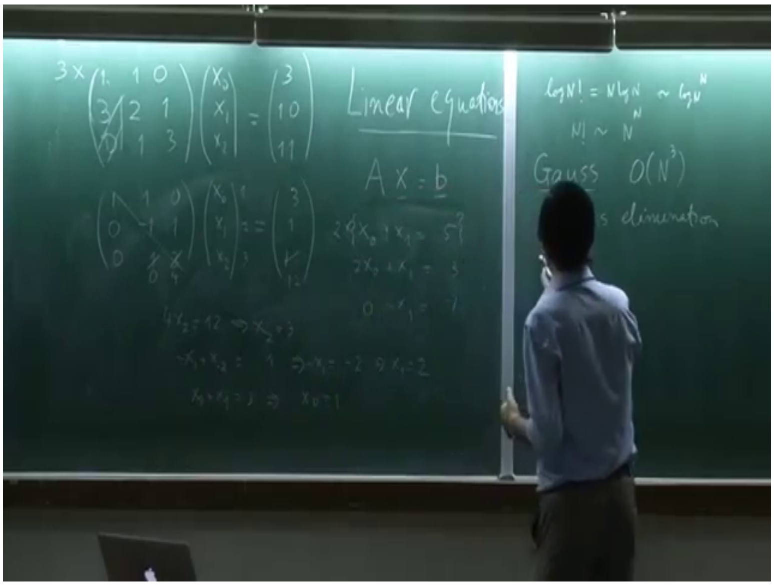


It is N log N, right sum factor plus. So, is N log N. So, this can be written as sorry if you. So, this is log of N to the power N. So, N factorial is order N to the power N; N factorial is huge N for N and (Refer Time: 06:07) which will crash if you will do to give 100 by 100 matrix; 100 tool bar; 100 is a big number. So, this is not a practical way to do it for large matrices; large means even 100 is low lower. So, they were of course, very clever people in and one of the cleverest person man nobody will doubt this, right.

So, Gauss gave us key and Gauss gives key in which you can compute N inverse in order N cube. So, not important, but out of the N cube; so, let us first do instead of computing A inverse, we compute let us try to solve equation. So, I will tell you the scheme. So, this is I have made a simplified matrix which I do not want to do a lot of algebra on the board. So, this matrix has been simplified. So, let us erase this stuff. So, this is not what we do in computer. In fact, this will illustrate among many other schemes which I discuss in the class that what you learn in mathematics is not exactly; what you use for computation; you have to come with a better scheme and these was not what we will put in computer, we do something different.

So, let us first look at the idea (Refer Time: 07:41) like in a upper diagonal matrix convert this to upper diagonal matrix.

(Refer Slide Time: 07:51)



So, suppose I have the equation x 0 plus x 1 is some number 5 2 x 0 plus x 1 is some number 3, it is always possible to eliminate this; how do we eliminate this, I can multiply this by 2. So, equation multiplying any number does not change the equation. So, multiply this equation by 2 then subtract this equation the new equation from this. So, this will eliminate 2 x naught; 2 x naught.

So, the second equation after elimination will become. So, this becomes 0 and x 1 minus 2 x 1 becomes minus x 1 and this one will be 3 times 2 is 10. So, 3 minus 10 is minus 7. So, the second equation is this I use a first equation to simplify the second equation. So, that is same this idea with Gauss is to Gauss elimination you eliminate few terms elimination. So, let us quickly work out what is done here. So, in this equation, I want to eliminate this term. So, I want to make it diagonal form upper diagonal form.

So, how do I eliminate this? So, I multiply this equation by 3 and subtract. So, what happens to the matrix by the way, I have to do the same thing here as well like I did here. So, multiply by 3 x naught x naught x naught is unknown. So, x naught should not be multiplied otherwise, there will be problem x naught is not to be multiplied. So, all the numbers 3 we have. So, let us first the first equation remains unchanged this is same this first one you do not do anything unless this entry is 0.

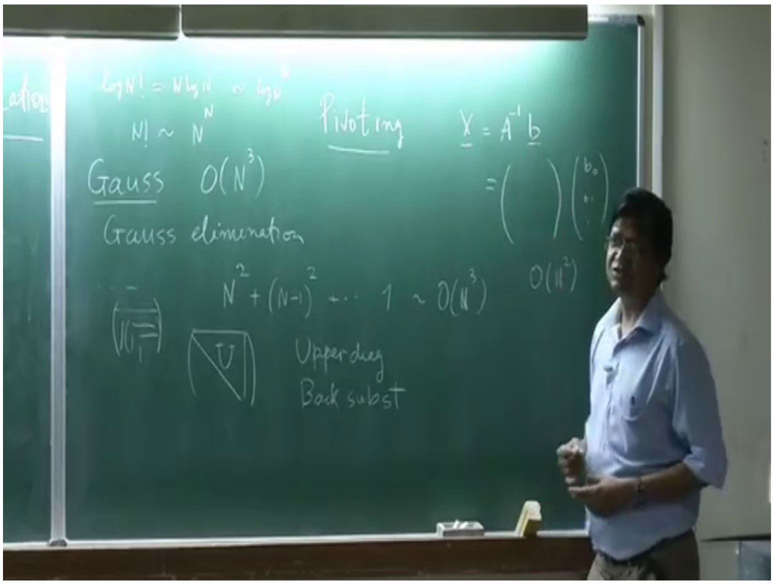
So, that I will discuss in a minute first (Refer Time: 09:59) and subtract. So, this becomes 0 what about this term 3 raise to is 3 times 1 is 3. So, 2 minus 1 is this one is unchanged because 3 times 0 is 0 and what happens to this nine minus 10 minus nine is one. So, and now I got up below (Refer Time: 10:25) the equation as I said; now I want to eliminate this one because this is diagonal eliminate one how to eliminate 1? Just add this equation. So, when I add what happens to this is minus 1 is (Refer Time: 10:51) 4 and this one is 1 plus 10 is 1 plus 11 is 12. So, this is my new equation, fine.

So, what is the last equation last equation is very simple 4 x 2 equal to 12 and we saw that what is the value of x 2. So, 4 x 2 is 12 implies x 2 equal to 3. So, here I eliminate it with this Gauss elimination. Now I found the answer to a upper diagonal matrix. The last entry will be only one entry and that is has only one unknown straightforward; next is now once I know x 2, then what is this equation minus x 1 plus sorry, yeah minus x 1 plus x 2 equal to 1, right this one and so, what should be the value of x 1 I substitute x 2 which is 3.

So, minus x 1 equal to 1 minus 3 will be minus 2. So, implies x 1 equal to 2 once for I know x 1 and x 2, then I can find x 0 from this top equation which is x 0 plus x 1 equal to 3. So, just substitute x 1 that gives you x 0 minus 1. So, my answer is x s are 1, 2, 3 that is my answer. So, this is how we solved. Now how long does it; what is the time complexity. So, the time complexity is very easy to estimate. So, imagine this N by N matrix. So, all these get rid of it. Fortunately, this is 0 here, it helped us a bit for me I did not had to do a lot of computation on the board; this (Refer Time: 13:04) the (Refer Time: 13:05).

So, I require N number of correct same thing to do. So, basically the first step when I make this.

(Refer Slide Time: 13:15)



This matrix below; this is N minus 1 by N minus 1 N square. Now I will replace this one by. So, this line remains unchanged, but I have to replace make the bottom one by let us N minus 2 by N minus 2 that will require N minus 1 squared same operation know. So, multiply this; I mean when basically you eliminate the first I eliminate this lines, then do the same thing; again eliminate these eliminate these. So, all the way up to one; so, this is how what is the order for this N square times N basically know.

So, is order N cube. Now there are factors in front which are important by the way order N cu say N cube and somebody makes it 0.7 N cube, it is a big gain is it a big gain or not a big gain 0.75; 0.7 N cube is 30 percent gain, we significant for super computers even 0.9 N cube is significant, but for estimation; I am not worrying about the factors, but there is a factor in front with, but first we need to reduce from N to the power N to N cube thus that is a very significant gain, but other gains are also significant, but not as much as this. So, this is how. So, this part is called Gauss elimination. So, I have converted this matrix A into upper diagonal matrix. this called U matrix upper diagonal this is a now.

So, this is Gauss elimination, but then after I had to keep finding x 0s x i’s. So, first find first one, then second last third last. So, this is called back substitution; back substitution. So, there must be 2 steps; first is Gauss elimination, then back step substitution now this is for solving x equal to b. Now only one h sometimes I may get these entry to be 0, it is possible (Refer Time: 15:50) now, then I cannot eliminate this right because I cannot multiply 0 multiply by any number is 0. So, what is done is you do some swapping. So, this equation is same as this equation; I can this equation go above and this equation come below.

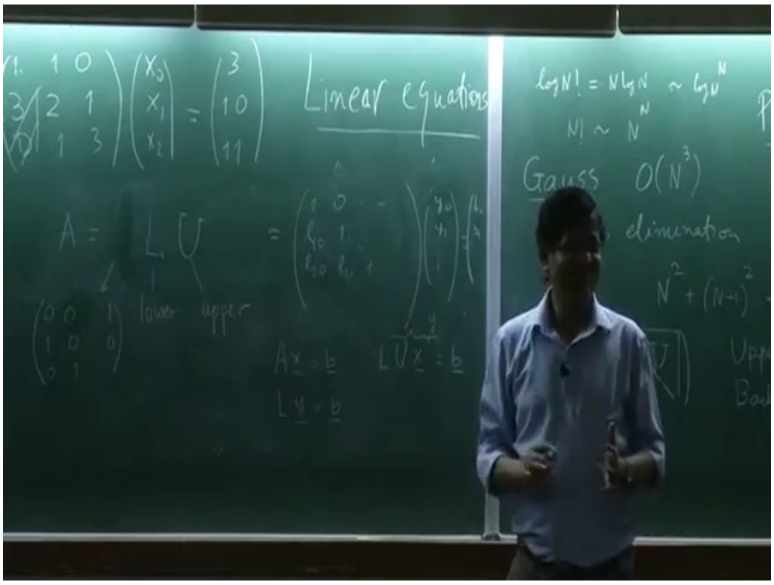
So, you swap. So, these are called pivots around the pivot, you do act action you know this is a here; you know for this operation, this is a main object. So, we want this not to be 0 hero cannot be 0.

So, this has to be come here and we use pivot. So, this is called pivoting. So, we have to make sure that the diagonal is non zero, but that can always be achieved unless there are like some anomalous could happens that none of the diagonals are 0s, but let us assume that does not happen. So, we can always swap. So, with pivoting and Gauss elimination you can solve this sub problems in N cube. In fact, this how computers solve it N cube now this way I can solve x equal to b, but like somebody says well I do not want to solve this equation, but I want to solve for b prime.

Now, I have to do the thing same thing again right x equal to b prime N order N cube again. So, better thing is to if you use this equation again and again rather if use this matrix a again and again for different bs, then get compute inverse and once you have the inverse then how many operations will you take its not N cube. So, I want to solve x equal to A inverse b. So, this multiplication matrix multiplied by a vector. So, how many operations? So, I had to multiply this number. So, always well it is very ideal b 0 b 1 like this. So, all these guys multiply here N operation, but they are N of these.

So, order N square. So, this operation is order N square order N square is cheaper than N cube. So, I would compute N A inverse for once and then use it again and again; now how to compute A inverse; now the idea which I will not teach in the class, but we do not (Refer Time: 08:40) take inverse by compute determinant, but a matrix A where there is a theorem.

(Refer Slide Time: 18:43)



You can always written as product of L times U L is a lower diagonal matrix lower and U is upper even L has a form all the diagonals are one. So, and L 0 0, no, actually L 0 1, I d not have any computer L 0 1, then L 0 2 L; what will that be no again a mistake; the L is of the how would you write L these are 0s this is first row the first index; then 0 next will be L 2 0, L 2 1, L 2 2 will be 1.

So, but always diagonal is one and upper diagonal has which I wrote this is up upper diagonal, but these are all not equal to one these could be not equal to one, but lower diagonal is always one. So, how many increase are there now in this L and U together the number of unknowns must be same as N squared right otherwise there is a problem you have more unknowns you cannot solve you have less unknown also you cannot solve.

So, number of unknowns will be square because this is diagonal plus upper; this is only lower L is only lower this is one now we can reduce A into L into U. Now to be precise sometimes, this pivoting is a problem. So, there is a matrix p; in front p has entries this for pivoting. So, computer adjust in such a way that pivoting is proper you do not have all this situation when there is 0 in the diagonal. So, this are of the form 0 0; there is only 1 1 here, it could be here, this could be here like this. So, this is for pivoting.

So, p is for pivot, but ignore it right; now you ignore it, if the matrix is good, you can always reduce it to L into U. Now it is again L and L and U are computed easy elimination now it is its more algebra, but its similar lines and I can do that in order N cube new computation can be done in order N cube once I have L and U then I can compute A inverse is that correct. So, you do not have to A inverse can be computed by L and U. So, let us compute given L and U how to compute x equal to b. So, let us assume that p is thus irritating it is that is not there ax equal to b; I want to compute, but somebody gave me a as L into U x equal to b.

So, I will call this as y reduce this to L y equal to b. Now again compute; now this is as long as we have diagonal upper diagonal or lower diagonal form you can do easily again back substitution, right. So, bottom one can be easily computed. In fact, the last entry is no sorry the top one you have to compute which one; top 1; x 0; no, y 0, y 1; b 0; b 1. So, how where will I start I know should not start from the bottom which should I start top what is the top of y 0 equal to b 0. So, I compute y 0 straight away in one shot, then put y 1 am when I going to find this I mean treble know.

So, y 1 will be L 1 0 y 0 plus y 1 equal to b 1. Now I already know y 0. So, I can compute y 1. So, you go from the top. So, I can compute y; how many operations? Order N square; it is a order N square because you see a always have N square by 2 numbers; we can compute this. Now once I know y, then I think I can compute x now. So, what is that U x equal to y, then x equal to y again this y. Now this will be like exactly like this back substitution; what it be for Gauss elimination? If you do that then I can get x answer. So, that is how we will compute x equal to b using L U order N square what about A inverse; given L and U can you compute A inverse?

Student: (Refer Time: 24:16)

Sorry.

Student: (Refer Time: 24:18)

That is right.

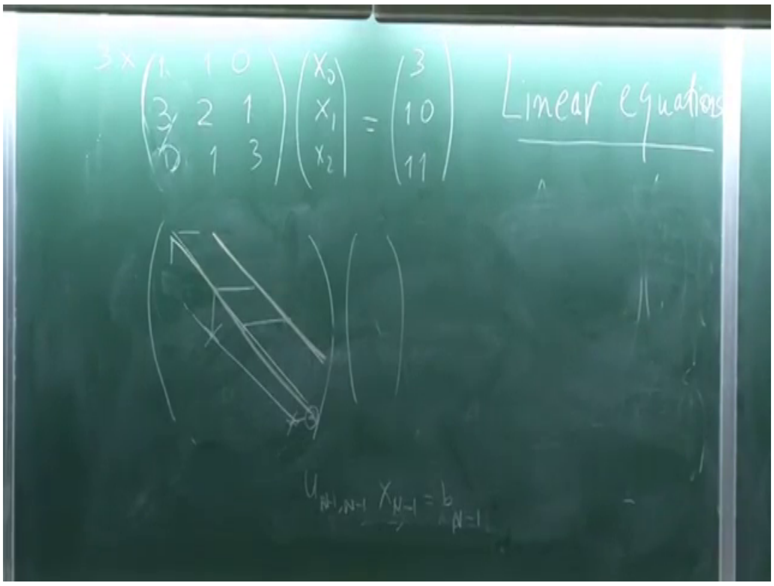
So, b; I had to choose properly. So, what kind of b as you have to choose. So, the to get the first column of A inverse I should choose as 1 0 0. So, that will give me x; x is you can do in the homework that is the first column A inverse second 1 is put 0 1 0 0 compute x that will be second column of a inverse. So, we will do it again and again for each column and that will give you A inverse. So, given L U; you can easily compute A inverse and that is order N cube; I mean all of these will order N cube. So, once you have N then you can solve for any b.

Student: (Refer Time: 25:13)

So, I did this quick succession; the Gauss elimination and L U decomposition of any matrix A can be decomposed and then how to find A inverse; now since we have done. So, far we can quickly finish one more algorithm of trio diagonal matrix. So, we did encounter this trio-diagonal matrices. In fact, this matrix is trio diagonal; I choose it that way it is. So, this trio diagonal matrix diagonal and one row upper the diagonal and one row below the diagonal. Now trio diagonal matrix you can do in or cheaper than full Gauss elimination.

In fact, I follow the same scheme. In fact, I did what here it works Gauss elimination for trio diagonal matrix 3 diagonals are this one 1 above; 1 below. So, suppose I have N by N matrix.

(Refer Slide Time: 26:23)



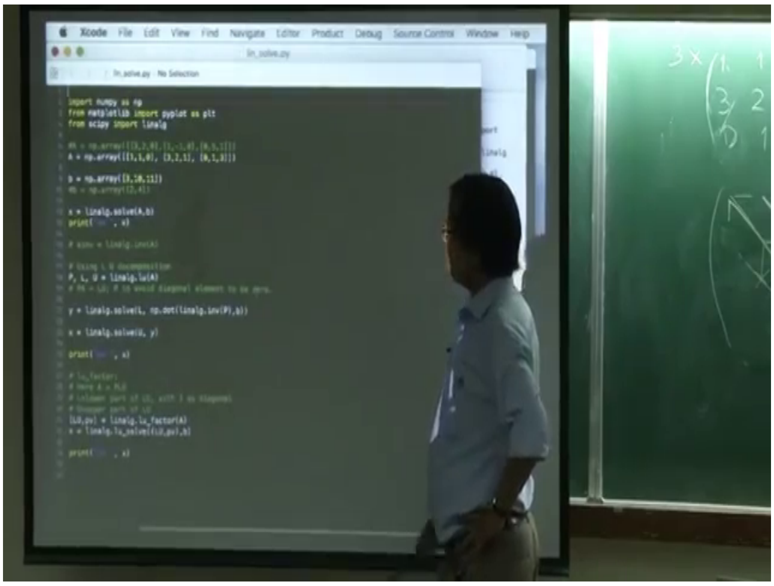
I have the diagonal one above and one below like this.

So, idea will be to eliminate this one and you will get an upper diagonal and upper diagonal I know how to solve it easily. So, do I eliminate? So, I do nothing with this next time I have 3 entries 1, 2, 3. So, I have to get rid of this how to get rid of these Gauss elimination. So, once I eliminate this I am left with this one; now I have 3 entries here what do I do eliminate then I get 2 entries.

So, each row will have only 2 entries keep cutting it and finally, the last one has how many entries last one has only one entry where the 2 entries I get rid of this; I have one entry. So, we get a matrix which is after this operation you get a matrix which is only diagonal and one diagonal. So, after Gauss elimination this one and this one and how many operations will it take its order N square; we can easily check its order N square actually order N square order N is order N is really cheap order N because I have to do only 1 1 1 elimination each time; 3 times or is order N. So, now, I can easily solve last one is easy no; last one is this entry upper N minus 1 N minus 1 multiplied by x N minus 1 equal to b N minus 1.

So, that gives you x and then back substitution. So, trio diagonal matrix is solved very easily, but you can write a very simple code maybe 5 lines and that will completely solve trio diagonal matrix pi python does a talk python has functions which will we do not need to write the functions it is done. So, I will show you how to; so, let us run these functions.

(Refer Slide Time: 29:14)

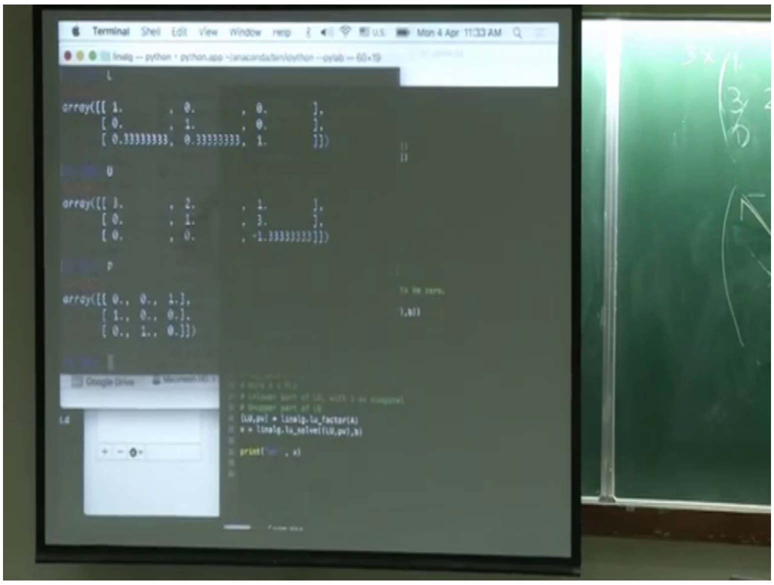


Let us first see linear solve. So, all these are part of linear algebra package of scipy. So, from scipy, I have to import linear algebra linear algebra this part of linear algebra.

Now, I write a matrix A which is same as this matrix I put b exactly what I solve and so, you have to solve functions; it takes arguments a and b; it gives you x we want L U, then you say the function L u. So, answer will come is P L U P is that I will show you what P looks like it is only has 1 1 in any row and using U; we can write exactly like what I showed for L U you can solve for x in 2 steps first of a y and then for x exactly; what I did on the board and I think we can this is another way which is L U factor. So, this you can ignore this can be done in one shot.

So, let us look at how. So, how to execute this one is that clear function syntax is trial. So, run.

(Refer Slide Time: 30:41)



I think it is Lin solver. So, our first; axis coming from first axis coming from this where I solved this one first one solve and second one is coming from this solution. So, let us look at what is A? A is this; what is L? L is this matrix L is lower diagonal. So, their diagonal is one and this one third and they also happens to be 0. So, is a simple matrix upper diagonal U. Now this cannot be. So, this is diagonal entry and upper diagonal I mean these are the 3 upper diagonal entries p is. So, computer has intelligently try to do a not pivoting it that for some benefits. So, p is not diagonal 1 1 1; it is 0 0 1 1 0 0 and 0 1 0. So, if I do L U.

So, dot product multiplication is not star. So, you do the dot product multiplication dot product. So, dot if L is dot A and x that should give b. So, where is A x matrix multiplication that should give us b. So, that is b 3, 10, 11. Now if I do dot of L and U; what should I get I expect it, but I will not get a it is stagnant a is switched. So, a switched see this one. So, this is gone above this is swapped. So, the row has been swapped. So, if I do dot of this P. So, P L U is A. So, I should dot this one with P. So, this is P L U and that will give you A that is same exactly same. So, this is how you solve for L U.

Now, the next equation is trio diagonal matrix. So, let us look at trio diagonal when a entry of this argument is slightly tricky here now the function we have to use is called solve banded. So, this not only trio diagonal, but any banded it could be 5 5 diagonals. So, I am using only 2 diagonal; 3 diagonal; one above one below and diagonal. So, the idea is here. So, if you have to look at this matrix. So, this one is upper diagonal and the sorry lower diagonal upper yeah upper first upper. So, upper 0 0 is you have to you have to give 3 numbers. So, only 2 are non zero right; all 2 are non zero here only 2 are non zero.

So, the first one is set to 0, it is 0. So, 0 1 1 the second one is all diagonal 1, 2, 3. So, 1, 2, 3, fine and third one is lower diagonal. So, 3 1 and there is 0 outside. So, this 0 is not part of the matrix, but python wants that it should be 3 by it should be order N length N. So, this is a 3 by 3 matrix, but this is not the; this mat this is not the matrix A; matrix A is this. So, argument I have to give is how many banded bands are there.

So, one above and one below; so, this is one for one of them is upper and one of them is below lower and this is A b matrix and b is a unknown; sorry, b is the right hand side as that will give me x. So, had it been 5 5 matrix some well bigger matrix with one more integer, it will below you have to trigger appropriately. So, this is how you give the. So, this is simple one, but you can also make quite big matrix and you can do entries here. So, you can run this. So, A b is not the matrix that is the only thing that I want to emphasize A b is not the matrix. So, then; so, this is my answer 1, 2, 3 1, 2, 3 is the answer x.

Now, A is a real matrix, but A b is not the real matrix. So, this is the diagonal part; this is upper diagonal with one of them not there; this is lower diagonal. So, this completes Lin linear algebra part of linear algebra; I will do one more thing, then we will we will stop this for solving x equal to b. Now another important factor functions are Eigen values you need Eigen values all the time.

So, python does offer nice set of libraries. So, this is for example, I mean this is triggle, but you can just use it given matrix A; you can compute Eigen value is an Eigen vector. So, it is that it will be simpler computer will do less work. So, this h is for. So, again it is part of the linear algebra package and I can this h is for Hermitian. So, you put any number as A. So, w will be the; I believe the Eigen vectors and this is the Eigen values; we will just check because I need to find one of them. So, this will be 3 Eigen vectors and there will be 3 Eigen values.

So, you know there are some tricky situations. So, my every matrix A which is N by N how many Eigen values can it have N always prove where those should be an Eigen values.

Student: (Refer Time: 37:11)

What?

Student: How does it remain (Refer Time: 37:13).

That does not degenerate yes, but why does it have N Eigen values.

Students: (Refer Time: 37:20)

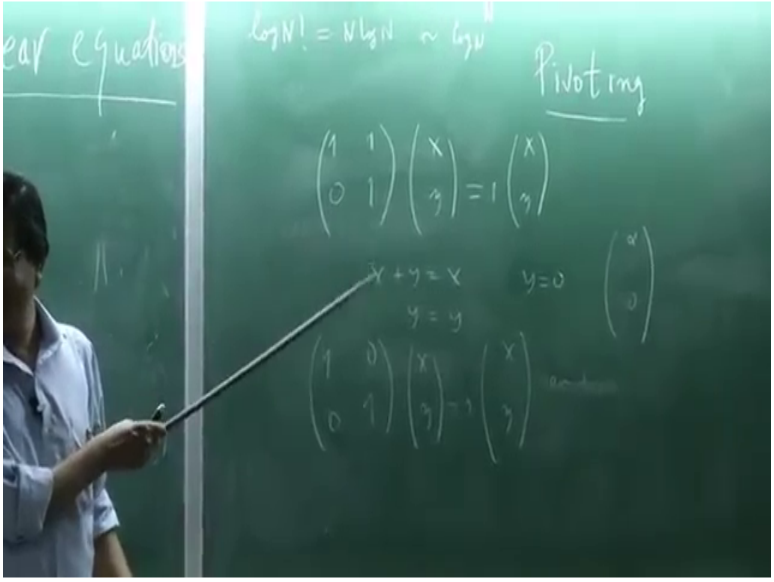
So the characteristic equation is Nth order; Nth order polynomial or N minus 1 highest exponent is N minus 1. So, it has N 0s what about Eigen vectors? does it is there guarantee that they will have N Eigen vectors.

Student: (Refer Time: 37:41)

No. So, on which situation there is no N Eigen vector I mean there is no guarantee of Eigen vectors what is the matrix 1 1 1 0; what you all think of this matrix this will have Jacobi form.

So, you have you can they are generalize Eigen vectors this one has only one Eigen vector. So, you can work it out x y.

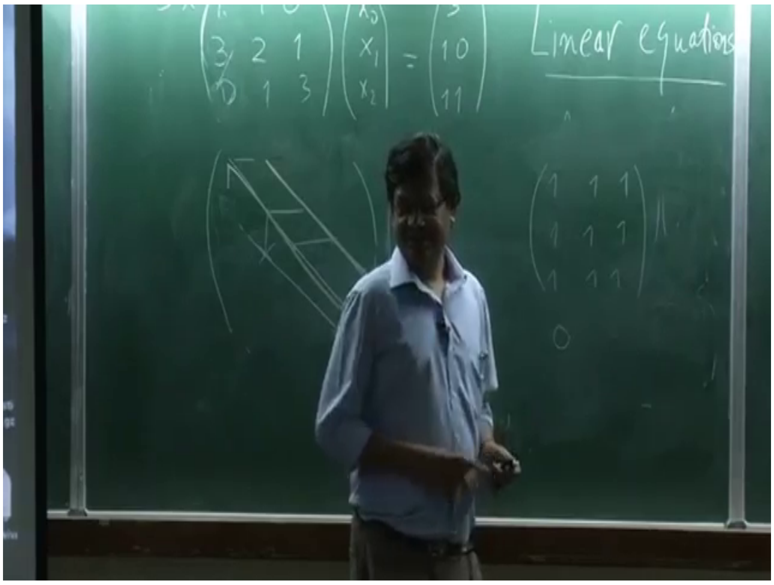
(Refer Slide Time: 38:10)



So, in vectors here Eigen values one degenerate. So, this has. So, 1 x y. So, there are 2 of them, but let me try to see whether I can get both of them. So, this x plus y equal to x and y equal to y. So, what does it tell you? So, y equal to 0 and x can be anything. So, the only Eigen vector I get is alpha 0. So, this is only one Eigen vector it does not have 2 Eigen vector along x axis contrast this with what about this matrix; one can say what about this matrix; how many Eigen vectors does it have; now this looks very similar no I accept this one; I made it 0.

So, if I do it x y is again 1 x y. So, x equal to x y equal to y; so, I get identity, but you can choose any 2. In fact, any vector any vector. In fact, any vector is Eigen vector for this identity matrix any vector is an Eigen vector, but then you have to choose only 2 linear independent. So, we will choose any 2 linear independent Eigen vector and this will work now this matrix. So, is that clear. So, normally in physics we do not deal with this kind of matrices quantum mechanics which is always Hermitian; this is non Hermitian matrix, but in dynamical systems we encounter this matrix. In fact, oscillator has this one of the examples because linear oscillator damped.

(Refer Slide Time: 40:26)



This matrix what is the determinant of this matrix. So, the matrix is now this is your matrix this is not computation.

Student: 0 0.

0. So, it will have 3 Eigen vectors not this one this is a counter example it has all Eigen values and all Eigen vector. So; what was the Eigen values?

Student: (Refer Time: 40:40)

Student: (Refer Time: 40:42)

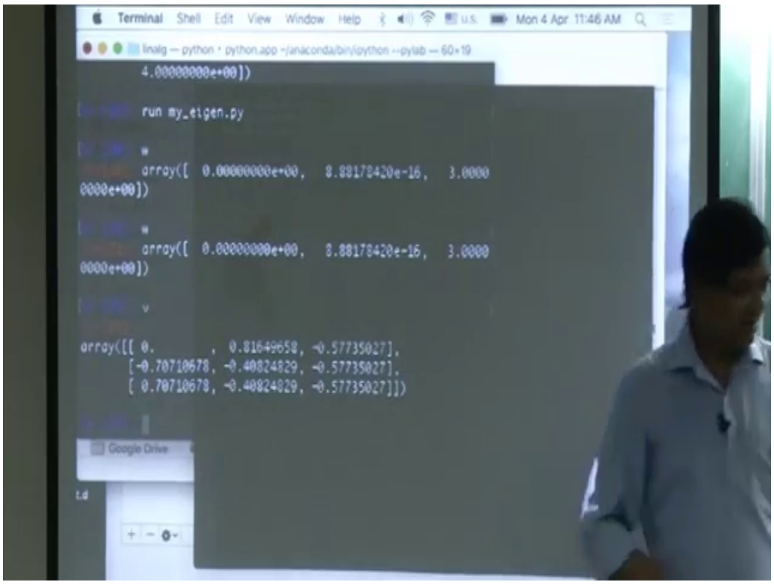
So, one of them must be.

Student: 0

0. So, product of Eigen value is determinant. So, one of them is definitely 0; other ones are; so, let us see we can work it out you prove this is the interesting Eigen vector. So, V and W; so, V is the Eigen vector and W is the Eigen values. So, I get 2 0s and one of them is 3. So, corresponding to 3 is equal to (Refer Time: 41:38) let me just.

So, 3 will correspond to 1, 1, 1; right. So, Eigen vector. So, this is x y z. So, what does 3 correspond to the Eigen vector corresponding to 3 1 1 1 will give you 3. So, 3 will give Eigen vector 1 1 1; it should have given actually.

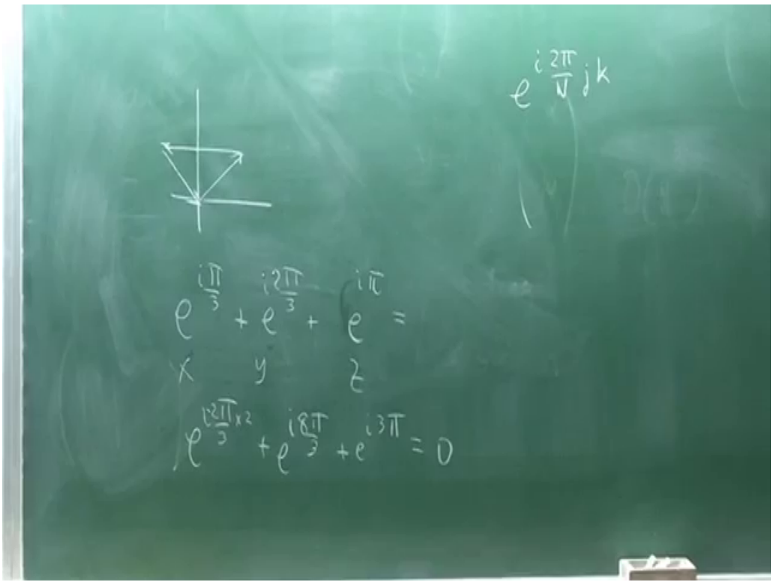
(Refer Slide Time: 42:04)



So, computation can I help you to come up with your guesswork and so, this is N W V. So, it is normalized. So, it is one by root 3 you know; it is one by root 3 minus sign does not matter this is the diagonal.

Now, these are. So, let us think of 0s I need some more space is that equal to 0, right; 0. So, I get x plus y plus z equal to 0. So, how can you satisfy this x plus y plus z 0 and in fact, there are 2 of them you know that 2 2 Eigen vectors the 2 0s. So, the 2 Eigen vectors. So, the idea is in fact, you know from your complex analysis that we start with let us see I did not think about this; I am just thinking about this one.

(Refer Slide Time: 43:13)



So, 60 degree is like this one and this one. So, this is complex vectors these are vectors. So, so this sum will give you 0. So, I want to just think of e to the power i pi by 3 plus e to the power i 2 pi by 3 plus plus plus 3 pi by 3 minus 1 e to the power i. So, this give you 0. So, this is minus 1.

So, I can make this x y and z these are Fourier transforms, right. So, e to the power 2 pi by N discrete Fourier transform. So, this is N. So, these are the solutions this is one solution. So, x, y, z; what is the other solution. So, e to the power i 2 pi. So, I give the 2 length into 2. So, remember what Fourier transform e to the power i 2 pi by N j k. So, just multiply by 2 or i 4 pi by 3, 4 into 8, pi by 3, then i 12, i by 3 3 pi. So, this is also gives you. So, there are 2 d independent solutions and this is how you can construct for any N by N matrix which are all ones and these are all real, but even these you get add and subtract. So, you have to do some more work to get these.

So, these please think about them and convince yourself that these are the solutions. So, due to lack of time; I will just stop. So, linear algebra I completed matrix normally you need something like 3 lectures. So, it is a good idea to show how to compute L U Eigen values are computed not again by this usual method it is something called q r decomposition. So, these are numeral scheme. So, it is called q r decomposition and the reference is the Newman is a good book. So, you can read if you like about Eigen values and Eigen vectors.