Symmetry and Group Theory
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Lecture No. 15
Matrix Eigenvalue Equation

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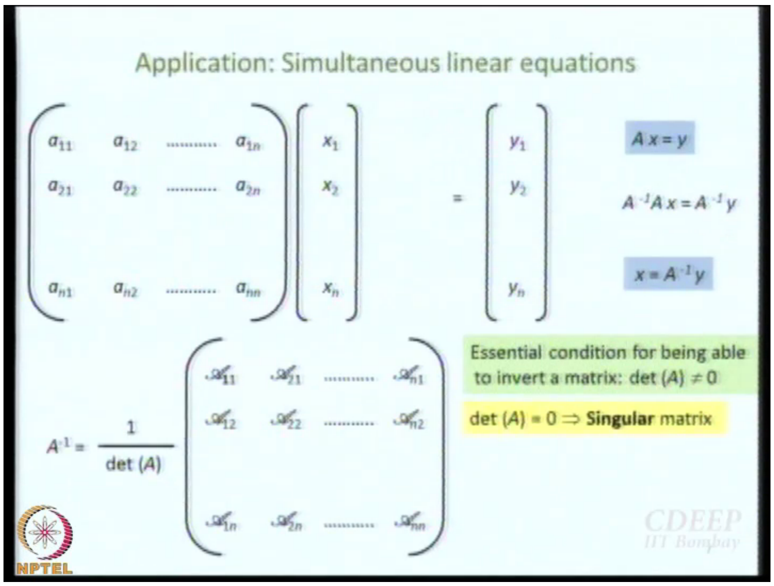

You all know what is eigenvalue equation is, what is eigenvalue equation? A Psi nothing to be shy about your function it is Psi, P S I right A operating on Psi gives small a factor multiplied by that is the eigenvalue equation what is the meaning of Eigen? Yeah, no, not proper one unique agent actually means unique. So, it comes from one is fine ok, a unique function and unambiguous function eigenvalue is unambiguous and unique function.

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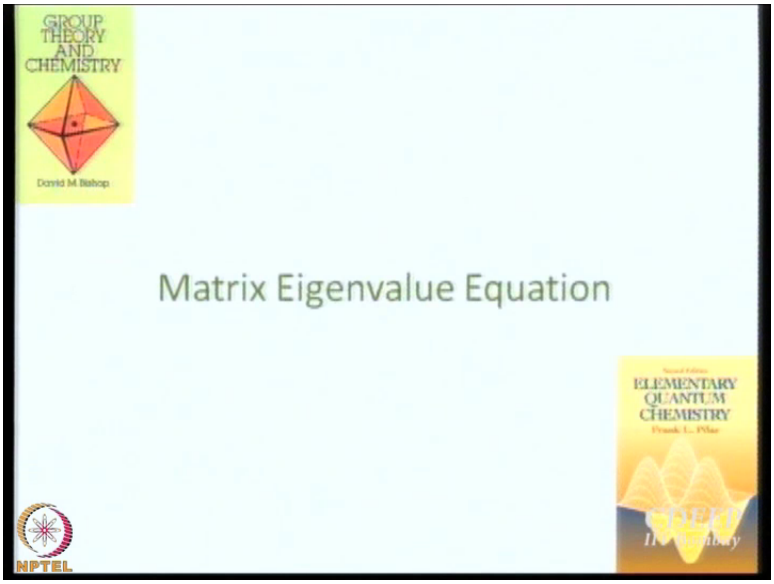

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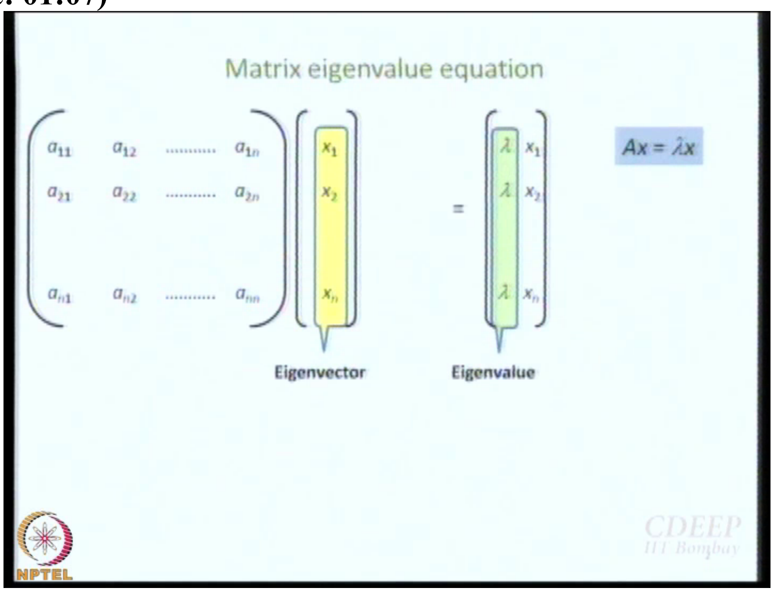

So, this is how the matrix eigenvalue equation is written right that was the mistake I have made these lambdas are all the same they will become different but that is for later not for now. To start with simplest form of matrix eigenvalue equation AX = Lambda X right, so the power is right. Lambda is one number for now it will become many number later on that we will see right, this is the way it happens. This column matrix is the eigenvector and the Lambda is called the eigenvalue ok for the square matrix which is n by n ok fine.

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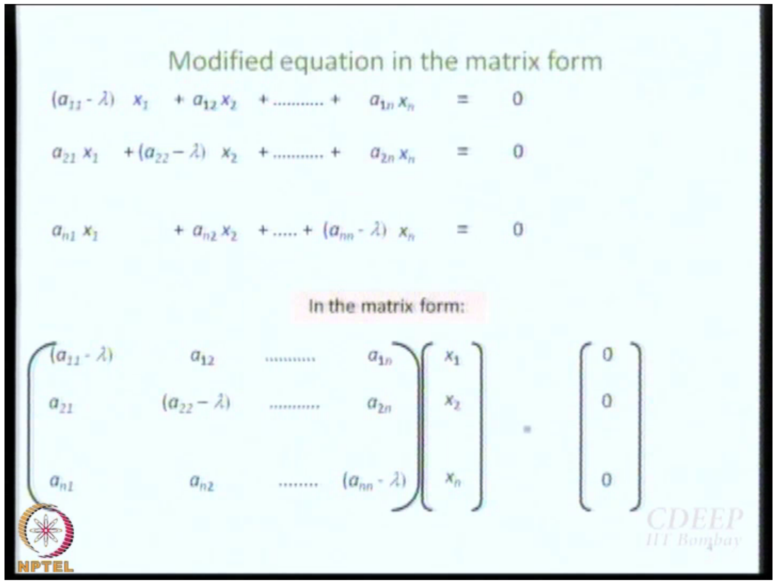

Now what we do is we can right it very simply as a set of simultaneous equation everybody knows this and if this is a matrix what will be the simultaneous equation what will be the first one a11 x1 + a12 x2 + etcetera etcetera then + A1n xn = Lambda x1 and the second one will be a21 x1 a22 x2 + so on so forth = Lambda = x2 right that is how you get the n number of simultaneous equations right these are the simultaneous equations for you right this is also Ax = Lambda x.

Now if you take the, if I make the right hand side 0 take Lambda X terms to the left then what will be the equations become what will the first one become a11 - Lambda whole thing into X1 + a12 into Lambda whole thing into X2 now then I am talking about the first equation now where did that 2 come from, 11 - Lambda whole thing into X1 + a12 - nothing into X2 + a13 into X3 so and so forth + a1n Xn = 0 ok. The only terms that get affected is the term in X1 right this is going to be the first equation. What will be the second equation will be a21 X1 + a22 -Lambda into X2 + so and so forth this is what it is? So what we see is something minus Lambda terms comes along the diagonal right.

You can right as many equations as you want when you get tired put dots and right the nth equation ok this is the set of simultaneous equation for you ok. Now if I want to right this modified equation in matrix form I think you will agree with me that this is going to be the matrix form very simple right. And this is a kind of matrix that actually occurs in many places in Quantum chemistry. Whoever have studied 425 might remember whoever studying 425 now will come across in few weeks time.

So this is the matrix the first 11 element is a 11-Lambda then a12 a13 up to a1n etcetera then a21 a22-Lambda then what is the third one, no, in this second row a23 or a 32, a 23 right then up to a2n and then you can right the whole thing and this is your matrix fine.

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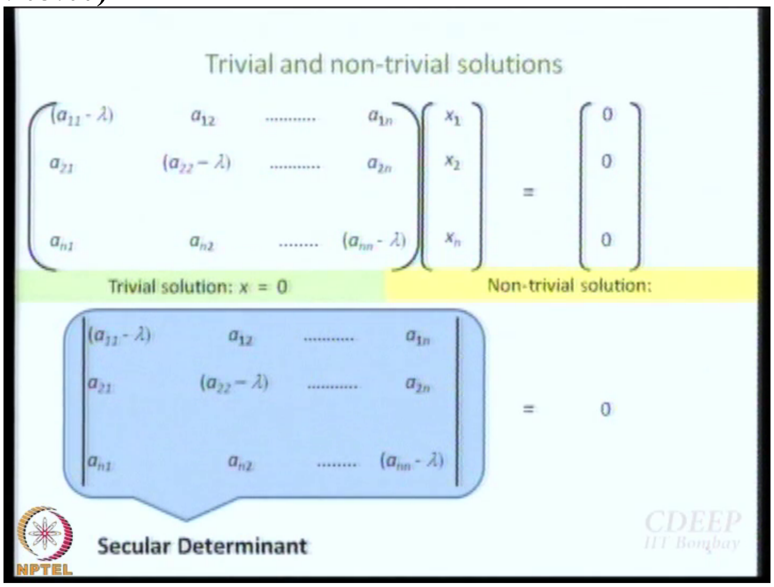

Now once you have this equation then you want to get the solutions what will be the trivial solution of this equation? X the matrix x = 0 right that is the trivial solution. What will be the non trivial solution that you cannot inverse the matrix right? If x is not 0 but you still get 0 what does it mean? Yes non trivial solution is the determinant equal to 0 and this is called the secular determinant right. Once again we are going to encounter this secular determinant later on in this course also but you can understand that if you have; if any significantly large then it is going to be a big determinant right.

Nobody wants to work with big determinants so what we will see it when you talk about bonding in organic molecules the big ones when say big maybe the naphthalene. Then you can actually cut the matrix into smaller blocks using symmetric considerations and that is called symmetric factorization of secular equations. So you are going to do that eventually right for now we just work with this as an abstract determinant secular determinant fine. Now you see secular determinant can be returned in interesting way.

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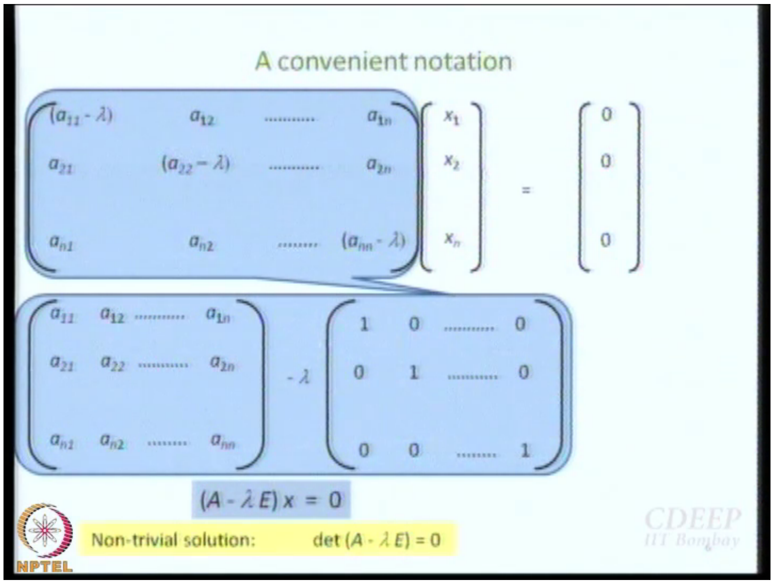

Shall we go back to the matrix equation what I want do is I want to break down this Matrix into 2 will you agree with me this is how we can write it, first you have the matrix A - Lambda multiplied by unique matrix does it not workout + all non 0 element of the unit matrix are 0, what am I saying half diagonal elements of the unit matrix are 0. Sometime I may say many strange things all half diagonal elements are 0. Only the diagonal elements are going to have the minus Lambda terms ok.

So I can write it in this fashion I can call it A - Lambda E into X = 0 alright. So the non trivial solution is going to be the determinant of A - Lambda E = 0 so far so good right.

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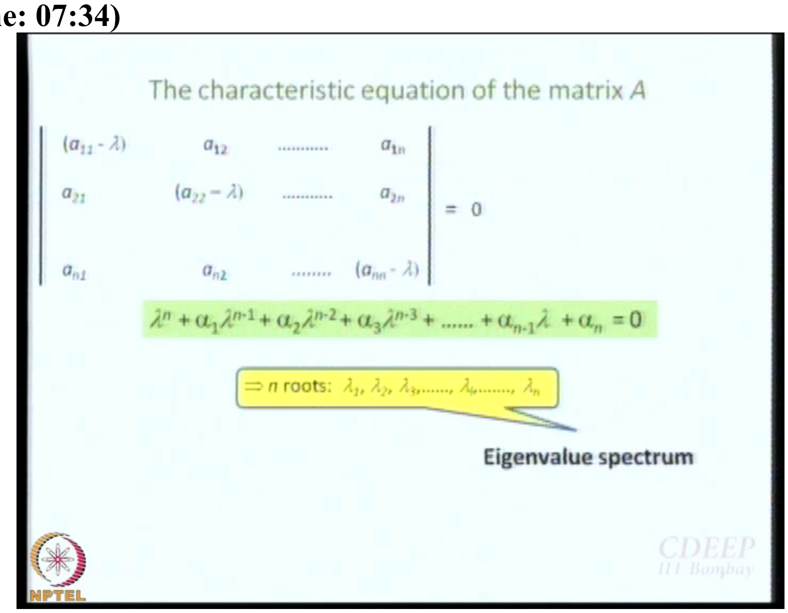

Now see here is the determinant this determinant has to be = 0 for non trivial solutions. Can you explain this determinant? Half say yes, half say no yeah any determinant can be expanded right if you have the; if you know whatever is there if you have the patience you can do it. It is just that it is written in a general form. Tell me if I expanded how many lambdas are there along the diagonal, n number of lambdas. What will be the highest order of lambdas in that equation, n. So which will be a polynomial in Lambda where the highest order is going to be n right. So, you are going to get the equation that it looks something like this Lambda to the power n + Alpha One to the Lambda n-1 alpha 2 to the power Lambda n-1 so on and so forth.

I do not know I was enthusiastic that I wrote so many terms but anyway finally you get second last term I want to right Alpha n-1 nth-1 Alpha multiplied by Lambda + you get alpha n. As a special case one or more terms name are missing that is a different issue is the general equation right. This is called the characteristic equation of the matrix A right. See what have we specified so far when you right when I write this equation what are the only quantities that can be specified a11 a12 a1n etcetera Lambda is a variable right I am trying to find the value of Lambda I do not know what it is.

Do I have x1 x2 etcetera here anywhere? No. The only thing I have is the matrix A so the solution that for Lambda that I get will be characteristics of the matrix A square matrix n by n matrix A alright. How many roots will be there n number of solution n number of roots Lambda 1 Lambda 2 Lambda 3 etcetera etcetera Lambda i and then again up to Lambda n right. Here we are going to get many values of Lambda n values of Lambda where n is the order of the matrix ok.

There will be total of n number of eigenvalue sometimes they can be equal to each other that is a different issue but nominally it is the n number of eigenvalues. And this n number of eigenvalues or set to span what is called eigenvalue spectrum ok eigenvalue spectrum. What does this mean? Can you take this story little further by yourself? I have a square matrix n by n square matrix what I am saying is that if I know the elements of the matrix then I can right on the character equation of the matrix and you are going to do that in few minutes.

And from that characteristic equation I am going to get n values of Lambda what is Lambda? Eigenvalue, so n by n matrix will have n number of eigenvalues can you say something more now something which I have not said yet. What is the next step hallow condition comes next just because you see spectrum you should not hallow conditions yet. Hallow condition will come after midsem. I have made a statement of eigenvalues can I make a statement about eigenvectors now.

What is the statement I can make, so I should have n number of eigenvectors also is it not, I should have a number of eigenvectors as well. N number of eigenvalue means n number of eigenvectors.

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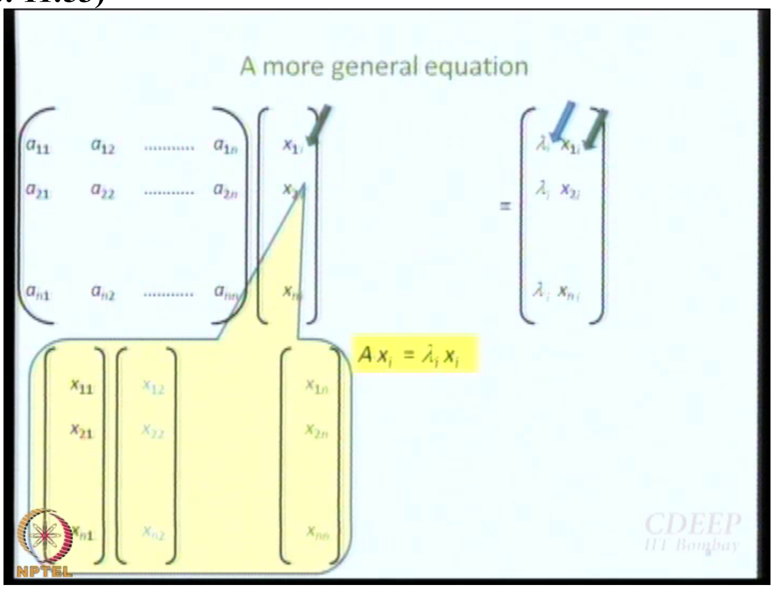

So now we need to modify this matrix eigenvalue equation a little bit to accommodate for the fact that you can have n number of eigenvalues and n number of eigenvectors right this is what we written earlier. Now what we have found is that Lambda is characterized by i so i can go for 1 to n if I write i is a substitute of Lambda I should write i as a substitute of X also right but at the same time I should not lose 123 all this things so it should come as a second substitute ok. What do you have in anyone eigenvector you have n number of X's right.

So number of those X is go from X1 X2 X3 X4 so on and so forth up to Xn right but then there is only one eigenvector. What I am saying is that I can have a number of eigenvector also. So I need a second quantum number if you want to call it, I need a second identifier right. So far this example i = 3 then this one is going to be second X of the third eigenvector. The first subscript the talks about the rank of X within eigenvector itself, the second subscript tells us about what is the rank of the eigenvector as well what is there roll number of the eigenvector.

Make sense do you agree that we need a second subscript for the access for the matrix element this is the matrix eigenvalue equation right ok. What is i? This is i, this is where I have written i,

what does i stands for? I stand for which eigenvalue it is. So you agree with me that there are n number of eigenvalue corresponding to each should I not have an eigenvector. Unique value is associated with the unit vector Eigen means one right.
So for eigenvalue number one I should have eigenvector number one also right wait. So that is why what I have do is instead of writing just Lambda I write i that for I think we are all in same page. Now what I am saying is that moment I write i it is not sufficient to right X1 and X2. Because X1 for Lambda 1 is not going to be the same for X1 say Lambda 3 that is why you need to use second subscript. So the first subscript tells you which row in the eigenvector your axis. The second value tells you which eigenvector it is so if you just go down you will see what is changing 1 2 3 4 up to n.

The first number changing the second number changing second number is i all the way so that is the identifier of the eigenvector itself. It is like a roll number what is your roll number 2014 then let us say 003 5 104 something like that. So 2014 is the year so for the entire population who have join into 2014 that 2014 is going to remind the same right. And 03 is department of chemistry that is going to be the same for all the students of department of chemistry but it is going to be 05 for electrical engineering.

And depending upon whether you are PG student or are integrated MSc student or 2 year MSc student next number will change. Show the different levels of identify these are identifiers. So you need the second identifier because we are going to have any number of Eigen vectors also Jeeva yes i = 1 is associated with Lambda 1, 1 number = 5 is associated with Lambda 5. What time now to say is that so now if I put in the i's AX = Lambda X is also not sufficient.

I should bring in either as well right and this is how it is written. AXi into Lambda I into Xi, what is A? A is the square Matrix that we are dealing with what is Xi? Xi is the ith eigenvector ith X matrix right. What is Lambda i? It is ith eigenvalue, Jeeva does that helps understand little bit ok. No we will work it out whether wait we are going to work out actually work out the eigenvectors today fine.

So now see for the different values of I, I am going to get the different eigenvectors X11 X21 up to X1n then X12 X22 up to X2n and so on and so forth last one will be X1 and X2 n X nn these are the eigenvectors, now whether it is little bit clearer right. I have forgotten your name Apoorva, no what is your name Shivangi it is ok fine. So now since it is clear let us make it serve it once again otherwise there is no fun right. Now what I want is do is this what do I have now I have n number of equations if I right it like AXi = Lambda AX i then for i = 1 to n.

For each value of i there will be one equation, who is going to handle so many equations. It is possible to condense everything into one equation. It is possible to condense the n number of eigenvalue equation to written into one equation. How do I do it now and without losing the information that there are n number of eigenvectors in number of eigenvalues how will I do it. What did you do earlier you have n number of simultaneous equation using matrix converted into one equation. Now what I am doing is combining the n columns into one matrix right that is square matrix holds beautifully but it was not square it would have been problematic.

You always multiply n by n matrix by another n by n matrix cannot you, that is why it is possible to right just a column one after the other construct a n by n matrix. Do you know what the solutions will be?

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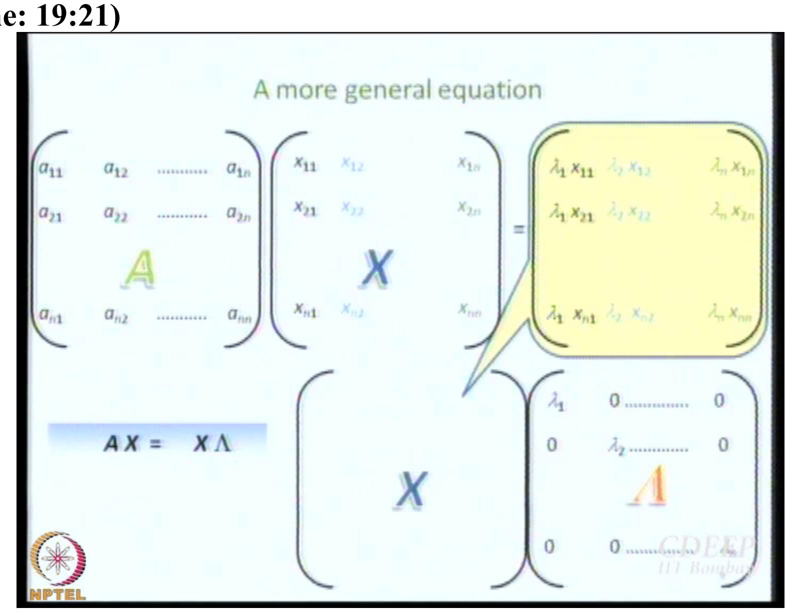

Solutions are also not difficult to understand after all if you neglect everything 1 2 and all that if you look at the first column that is a first eigenvector right. What should the first column in this matrix be Lambda 1 multiplied by the first eigenvector ok, are we ok with this? This is my first column Lambda 1 X11 and the second row is Lambda 1 X1 and so on and so forth until the last one is Lambda 1 Xn1 Lambda 1 remains the same just a matrix eigenvalue equation.

Similarly the second column will be unless you will have a second Eigenvalue equation will be and so on and so forth until the nth column right. What I am able to do that I can able to take those n number of equations and combined them into a single matrix equation right clear, so if it is clear then again try to make it as a habit. Let us do it like this I multiply two matrix fine I got one matrix now I want to see whether I can write this product matrix as a different product then it will be fine.

Let us say this matrix name them over A now the second Matrix what was I calling the second matrix the eigenvectors that is small x. Now instead of small x let me right big X because this matrix is bigger than the constitution matrices since write small x we will write big X ok. What is the right hand side?

Left hand side is very nice AX right hand side what I want to do it I want to split this as a product of two matrices and I want one of those matrices to be X, I have given the half the answer first one is X, what will be the answer for the second matrix be purgative, in one row ok let us see what happens. This is first row multiplied by first column 1 by 1 element will be Lambda 1 X11 fine what will be second one do you get Lambda 1 X21. So I think we got the right answer for the first one this is what it is going to be this is going to be the Lambda matrix.

A diagonal matrix where the diagonal element is this is defined lambdas all diagonal elements are all 0's you multiply C4 with yourself how it works, it works right this is your Lambda matrix AX = AX Lambda ok. So now I can taken care of fact that there are n number of eigenvalues. I taken care of the fact that there are n number of eigenvectors and I have been able to combine everything in single equation and write very simply AX = X Lambda do not forget AX and Lambda all are matrices and they are all n by n square matrix.

Anyway be like to work with square matrices all the time because they are very easy to handle ok fine. Now let us see if we can make it little more simpler. If AX = X Lambda so you see if I left multiply by X inverse what will happen? On right hand side I have only Lambda. What will have in my left hand side I have the similarity transformation which is also nice right let us do that, are you ok with this. You right AX = X Lambda then if I left multiply both side with X inverse and of course with what you multiply left multiply or right multiply is all the matter of intuition.

You can see easily left multiply by X inverse the right hand side X inverse gives you unit matrix ok anyway it is very simpler. And then you do that very nicely left hand side becomes the similarity transformation of A with X. So see now we are inching closer to figuring out what actually the values of Lambda AX are. In any case better know A is, if I do not know about A then what I am talking about. So if I know A and if I know the eigenvector matrix then I can perform a similarity transformation of A using the eigenvector matrix and get all the Lambda values in one shot.

What is this process called? Diagonalization starting with the non diagonal matrix I have found a way of getting the diagonal matrix by similarity transformation. Moreover what the diagonal matrix gives us that it gives us all the n values of Lambda at one shot, is it not, Lambda 1 Lambda 2 etcetera etcetera up to Lambda n. If I know A and if I know X as we will see actually it works the other way now. We actually determine the Lambda first and then we try to find x.