**Computational Chemistry & Classical Molecular Dynamics**

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**Lecture – 18**
**Matrix Diagonalization and Similarity Transformations**

Hello and welcome to this next lecture of computational chemistry. In the last lecture we were considering matrix Inversion we defined the inverse of a matrix which involved co-factors as well as the determinant and using that we worked out a strategy. How to convert all the non-diagonal elements to 0 and how to make all the diagonal elements to 1 by dividing by the appropriate numbers in the diagonal values.

And if some diagonal values were 0, we exchanged that particular row by some row below that diagonal which has a large value in the diagonal term and replace it with a new row which is a non-0 in the diagonal. So, we were considering the program and we shall very soon consider that program also but before I go into the program for matrix inversion, I want to describe another important topic which is called matrix diagonalization.

So, in this process of matrix diagonalization you convert a matrix usually a symmetric matrix n/n matrix into its diagonal form I shall illustrate that with a 2/2 case which I am considering in this example now let us look at this example of matrix diagonalization.

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## Matrix diagonalization (CONTINUED)

- $A\vec{X} - \lambda\vec{X} = (A - \lambda I)\vec{X} = 0 \qquad (1)$
- $\det(B) = \det(A - \lambda I) = 0$ for non trivial (non zero) solutions

n × n matrix, $\det(A - \lambda I)$
is an $n^{th}$ order polynomial in $\lambda$
the n roots of this polynomial are the n eigenvalues.
By substituting each eigenvalue in Eq (1)
We obtain the eigenvector corresponding to that eigenvalue.

What this has is A is a matrix and X is a vector X is a column vector, so the matrix A multiplies the column vector and the result of that operation is nothing but lambda times the column vector The equation is AX=lambda x that is my equation or AX– lambda X=0 that is my equation. This is called an eigen value equation so what is the meaning of this equation? X is some vector and when you multiply on the left of that vector.

It is a column vector by matrix A what you get is again that column vector multiplied by a constant so that means if X was a vector in some direction okay the multiplication of a matrix gives you a multiple times the same vector. So that means multiplying by that matrix has not changed the direction of the vector. So, in general when you multiply by a matrix A on to a vector X its direction also changes.

So this is a special case where the direction does not change so then the question would be how many vectors are there which will not change directions when I multiply by the matrix A it turns out that if A is an n/n matrix there will be only n vectors like that if A is 10/10 matrix there will be only 10 vectors independent vectors which will not change directions so this therefore these vectors are called eigen vectors.

And the values are lambda are called eigen values so this particular problem is called an eigen value problem so what is the problem of matrix diagonalization you find out all the diagonal values are nothing but the different lambda values. Find all the lambda values which satisfy this equation, so I can rewrite the same equation as A–lambda i*X = 0. What did I do? I just instead of there is an AX.

So, when I multiply this out A * X that is the first 1, then the next 1 will be lambda*i*X where i is nothing but a unique matrix so whenever I have a lambda X here, I can always insert a unique matrix in between because it will not change anything unique matrix can be inserted anywhere without any change of the product, so this is 0 which means our matrix here A– lambda. This is a matrix that operates on X to give me 0 now there are only 2 possibilities.

Because on the right side I have 0 either X is 0 and this is 1 possibility or now the determinant of A– lambda I that has to be 0. So, if the determinant of this matrix is not 0 then what can I do? I can get the inverse of A–lambda I if I get the inverse of A – lambda I and multiply on the left by that inverse so that inverse*A– lambda will be 1 correct so 1*X will be 0 so then X has to be 0 so that means if the determinant of B is not 0 then I can get an inverse matrix.

Then it will force me to say that X will be identically 0 so the only way this has a equation solution if the determinant of this is = 0 so only for a 0 determinant there will be a no inverse matrix. So, I will get a non–trivial solution for the value of X. X is an eigen vector so now let us consider this determinant of A–lambda I. What is this A– lambda I? It will be an n/n matrix so if I have A–lambda I when I expand the determinant.

So, that determinant will be an nth order polynomial in lambda. It is a nth order polynomial in lambda an nth order polynomial in lambda will have n roots, so lambda will have n roots and those of this polynomial are called eigen values so once I know the eigen value by solving the polynomial equation I can substitute that eigen value back here and get that A*X and lambda*X once I know the lambda, I can satisfy this equation.

So, therefore once I know the eigen value lambda I can know the eigen vector as well, so this is what is illustrated in my next slide. So, we will illustrate this for 2/2 case it is a very easy case so once we understand the easy case, we can understand all complicated cases all other things will be exactly similar, except the polynomial order will be larger there will be more and more eigen values now consider the details of a 2/2 case.

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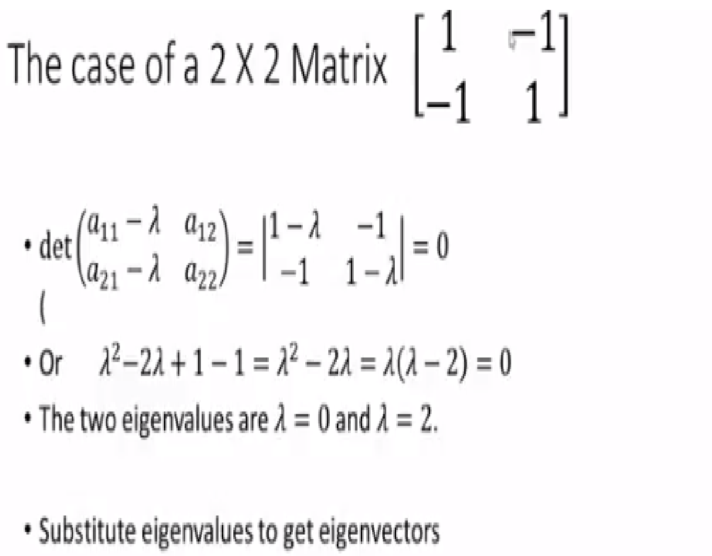


That is what I have given here so these are 2/2 matrix what is my matrix? 1 -1 -1 1 this is a 2/2 matrix so now I want to find that eigen values of that. What did we conclude from the previous slide? The determinant of A–lambda that should be 0 so what is A–lambda so from this particular metrics so I have to subtract lambda from all the diagonal values. So here, there is an error here.

It should not be a11 – lambda a12 a21 a22 – lambda so this lambda is in the wrong place. Please make sure that this - lambda comes into 2 nd term here. Okay, so what is my determinant a11–lambda a11 is 1 so it is -1 lambda -1 remains the same. a21 -1. There is -1 so there is no - lambda here. This is not correct so this - lambda should go under second term. So this a22–lambda my a22 is 1.

This is a22–lambda = 0 so I have to calculate the determinant how do I get this determinant to get this determinant suppose I have a, b, c, d, what is my determinant? a c – b d so that is what I have given here. The first term in the determinant would be 1–lambda*1– lambda so that is 1 - lambda squared so what is 1-lambda square lambda square–2 lambda +1 this is 1 - lambda square.

Okay and what is my second term? 1-lambda square - this * this so -1*-1=+1 so I have to take 1 more - because in the determinant. The determinant is a product of these 2 values - the product of these 2 values. So, since this -1 so this is my equation lambda square–2 lambda+1-1 okay so what is that now? 1 and 1 cancels so it is lambda square-2 lambda this is 0 so when lambda square–2 lambda=0.

I can write it as lambda*lambda– 2=0 this is the same as lambda square -2 lambda so what do we conclude from this now this is written in terms of all the roots of that equation, so this lambda is nothing but lambda–0 so this product is lambda-2*lambda–0 because when I say lambda is nothing but lambda–0. So, these are my 2 roots lambda-2 means lambda-2 is a root just lambda appearing lambda = 0 is the root.

So, this product implies that either lambda =0 or lambda =2 so these are my 2 roots of my polynomial equation and from what I concluded in the previous slide is that both these are eigen values. Now I have to substitute these eigen values into my matrix to get the eigen vectors that is what I shall do in the next slide.

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For $\lambda = \lambda_1 = 0,$

- $\begin{pmatrix} a_{11}-\lambda & a_{12} \\ a_{21} & a_{22}-\lambda \end{pmatrix}\begin{pmatrix} X_{11} \\ X_{21} \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} X_{11} \\ X_{21} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$
- $X_{11} - X_{21} = 0$

$-X_{11} + X_{21} = 0$

or $X_{11} = X_{12}$

we can take the first eigenvector to be

$$\begin{pmatrix} X_{11} \\ X_{21} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Any multiple of the eigenvector is fine

So, now I shall get the first eigen vector so to get the first eigen vector what I do I substitute lambda=lambda1=0 remember I had 2 values of lambda so for the first eigen vector I am going to substitute lambda 1=0 so that is a11 - lambda a12 a21 a22 – lambda here it is incorrectly now this into X okay a - lambda X = 0. So, when I multiply this, I should get 0 and 0 and this is my product 0 and 0.

Because this is a matrix a and it operates on a column vector, so I will get a new column vector what is my new column vector? This is 0 column vector so now there is 1 special change I have made here remember earlier I have X1 and X2 that was there before now why do I have it X11 X21 because there will be 2 eigen values lambda 1 and lambda 2 and for lambda 1 this my eigen vector.

X11 and X21 this my eigen vector for lambda 1 for lambda = lambda 2 I shall use it X21 and X22 because the 2 nd label in my column vector here represent which lambda it corresponds to so since there are several lambdas, I need the 2 nd particular column here. So, now let us multiply through this and now we know that lambda was identical 0 so what is the rest of it? 1 -1 -1 1 this is my original matrix lambda = 0.

There is nothing to subtract that into X11 and X21 and that is = 0 so how do I expand this now this expansion is using the matrix multiplication so first row i multiply by the 1st column so what do I get? 1 * X11 this is my X11 then -1*X21 and this is –X21 that is 0 because this particular row into this particular column is 0. So, this is my 1st equation and what is my second equation? -1 * X11 1 *X21 that is –X11+X21 = 0.

So these 2 equations I got by expanding and multiplying this matrix now you see that both these equations are identical why are they identical? Because this is X11 –X21 = 0 just take the - of that thing minus of this equation is –X11+X21=0 since both these are identical the only solution to this is X11=X12 this is my solution because the sum is 0. So, once I know that X11 = X12 this I will call as the first eigen vector.

So I want to write the first eigen vector as a column now X11 and X21 now I am taking this as 1 and 1 so I am taking this as 1 and 1 now you will ask me why am I taking 1 and 1 and why I am not taking 2 and 2. It does not matter if lambda is an eigen value so if you multiply both by a constant it does not change anything the direction does not change by multiplying by scaler. So, if lambda is an eigen value I can multiply both sides by some lambda, so it will not matter.

So I can take 1 and 1 as an acceptable solution so this is my first acceptable solution 1 and 1 so a multiple of this eigenvector is fine because since X 11= X12 1 and 1 is okay 100 and 100 is okay million and million is okay only thing it should be finite, and it cannot be 0 because if it is 0 again it does not mean anything. So, it should be either a non negative number so there is my non negative finite number so non 0 finite number.

So, this is my first eigen vector now how do I determine the second rector? Let me pause give you time to think about it so instead of lambda = lambda 1 I have to substitute lambda = lambda 2 so that is what I will do in the next slide.

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For $\lambda_2 = 2$,

- $\begin{pmatrix} a_{11}-\lambda & a_{12} \\ a_{21} & a_{22}-\lambda \end{pmatrix}\begin{pmatrix} X_{12} \\ X_{22} \end{pmatrix} = \begin{pmatrix} 1-2 & -1 \\ -1 & 1-2 \end{pmatrix}\begin{pmatrix} X_{12} \\ X_{22} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$
- $-X_{12} - X_{22} = 0$ $\quad$ $-X_{12} - X_{22} = 0$
- $X_{12} = -X_{22}$ $\quad$ $\begin{pmatrix} X_{12} \\ X_{22} \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

The matrix of eigenvectors is

$$X = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Now look at this for lambda 2 what is lambda 2? lambda 2 was value 2 so now I am going to subtract 2 from the diagonal term a11 – lambda a12 a21 a22- lambda so this is written correctly here always subtract lambda from the diagonal values so when I substitute that now I need a new eigen vector what is new eigen vector? X12 X 22 remember in the last case I wrote it X11 and X21.

Because that corresponded to the first eigen value now since the second eigen value I have given the second subscript I have made it = 2 so a - lambda into a new eigenvector now that again is = 0 so now what I shall do in the matrix. I shall subtract -2 from the 2 diagonal terms so what is my new resulting matrix now? My new resulting matrix would -1 -1 -1 -1 all 4 are -1 so what is my equation now? –X12 –X22 = 0.

And from the second 1 also I get identically the same equation –X12 – X22 = 0 so what is the solution of this equation now, so solution of this equation is X12 = -X 22 since –X12-X22 = 0. 1 has to be – of the other then only the sum is 0 so what si my new eigen vector now my new eigen vector is 1 and -1 now I have 2 eigen vectors now the first eigen vector was 1 and 1 and second eigen vector is 1 and -1.

So, I can combine all the eigen vectors into a matrix of eigen vectors so since a was 2 by 2 matrix my matrix of eigen vectors is also a 2 by 2 matrix if I had a 10 by 10 matrix a my X also there will be 10 eigen vectors and 10 columns so I will have a 10 by 10 column matrix 10 by 10 matrix of 10 eigen vectors. Now we will introduce a new concept using these eigenvectors I can multiply the matrix a in such A way that I get that diagonal value.

So that is my next slide now look at the next slide.

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## Diagonal Matrix (Similarity Transformations)

- $X^{-1} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & -1/2 \end{pmatrix}$

$$X^{-1}AX = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & -1/2 \end{pmatrix}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}$$

$$X^{-1}AX = A_D, \qquad A_D = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & . & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & \lambda_n \end{pmatrix}$$

So what am I doing? Since I knew the matrix X I can get the x inverse of the matrix X so how do I get the X inverse? You already know that the inverse values are co- factor of element aji divided by determinant of A so what was my determinant of a go back and see.

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For $\lambda_2 = 2,$

- $\begin{pmatrix} a_{11}-\lambda & a_{12} \\ a_{21} & a_{22}-\lambda \end{pmatrix}\begin{pmatrix} X_{12} \\ X_{22} \end{pmatrix} = \begin{pmatrix} 1-2 & -1 \\ -1 & 1-2 \end{pmatrix}\begin{pmatrix} X_{12} \\ X_{22} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$
- $-X_{12} - X_{22} = 0$ $\quad$ $-X_{12} - X_{22} = 0$
- $X_{12} = -X_{22}$ $\quad$ $\begin{pmatrix} X_{12} \\ X_{22} \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

The matrix of eigenvectors is

- $X = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

What was my determinant 1*-1 is -1 *-1 the determinant is -2 the determinant of this is -2 I shall use that to get inverse of X so what is the inverse of X ½ ½ ½ -1/2 this is the inverse of my matrix X now how do you know that these are inverse of matrix X? The best way to check is multiply X inverse *X. When you multiply X inverse to X you should get identity matrix then only you know that it is inverse of X.

So, what am I doing now? I am going to use a technique which is called a similarity transformation I have obtained X a matrics of eigen vectors X inverse is the inverse of the matrics of eigen vectors. So, I shall multiply this is my matrix A I multiply on the left by X inverse and on the right by X so this my X inverse A * X when I do this particular product of these three matrices.

What I get is 0 2 0 0 so what are these 0 and 2 and these are nothing but my eigen values I started with so what we found here is that once I have a matrix of eigen vectors I have an original matrix A and again remember I am taking a n by n matrix I found it eigen values I found it eigen vectors found is eigenvector matrix X inverse AX this is called a similarity transformation whenever I have a matrix A and I find its vector of matrix of eigen vectors.

When I do the X inverse AX it is called a similarity transformation when you do a similarity transformation on any matrics what you get is the diagonal values of the eigen values all the diagonals values will be eigen values off diagonal values will be 0 so this means I have converted A in to its diagonal form of the matrix using a similarity transformation, so I have generalized it to any matrix of any size.

Take a matrix A of any size find its eigen vectors find the eigen vector matrix find the inverse of eigen matrix X inverse AX is A in the diagonal form so what is the diagonal form of matrics? The diagonal form will be all the diagonals values will correspond to the eigen values of a matrix all the off diagonal values will be 0 and once you have a diagonal matrix it is very easy to calculate the determinant.

The determinant of a diagonal matrix is nothing but the product of eigen values now we will see that if the determinant of A is 10 the determinant of A diagonal also has to be 10 because it is multiplied by 2 matrices X and X inverse so if X has a determinant of value alpha X inverse will have a determinant of 1 by alpha because X inverse* X is 1 so the determinant of X inverse will be 1 by determinant of X.

So, automatically they will cancel so the determinant of A will be identically the determinant of A diagonal values so now what we can do we can try to have a strategy to calculate the eigen values and eigen vector by some program that is our next strategy.

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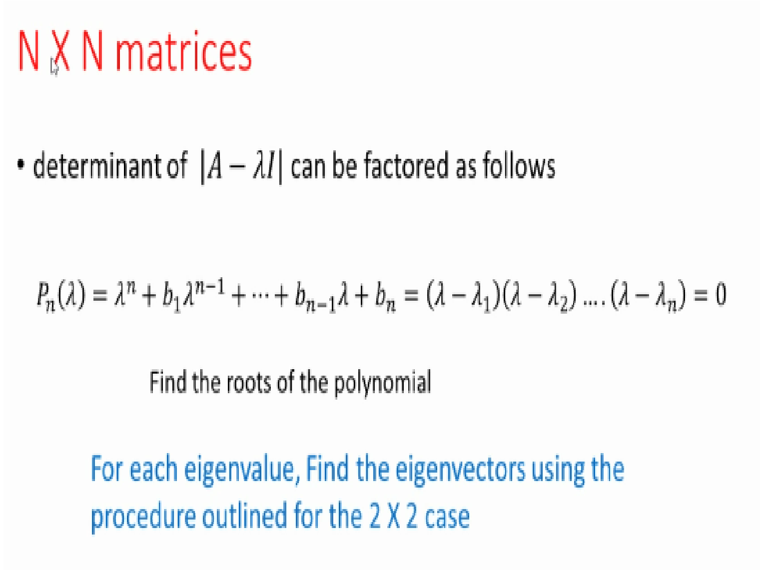


So, before I go to that when I have an n by n matrix that determinant of that n by n matrix that is the determinant of A–lambda I can be written as a polynomial. It is written as a polynomial of the n th power of lambda because when I expand A - lambda I and A is a n by n Matrix so n th power of lambda will occur, so I have written that determinant now as a polynomial lambda to the n b 1 to the lambda n-1 all the way upto bn.

So, this entire polynomial now and this particular polynomial this is the normal form in which you write a polynomial, but a polynomial can also be written in terms of its roots so n th order polynomial can be written as a product of these functions which are these functions now lambda -lambda 1 lambda-lambda 2 and up to lambda – lambda n so all these lambda 1 lambda 2 lambda n are the roots of that equation.

So, every polynomial equation of n th order can be written as a product of factors in which each route is contained so these are very fundamental statement in your polynomial equations or Algebra, so a polynomial can be expressed as a product of the n roots of the polynomial where each root is subtracted from variable lambda, so these are my n roots and for each eigen value now which is a root.

I can find that eigen vectors using exactly the procedure that I gave him the previous slide I use exactly the same procedure substitute the value of lambda then a-lambda x=0 and I get relations between all the excess when I get the relation between all the excess, I value I find the values of the eigen vector so next what we consider now we will briefly consider how to write a program to calculate these eigen values.

So, in the last class we discussed a program for inverting the matrix in this class we want to discuss a program to get the largest eigen value so finding eigen values is a rather complex program so what we shall do we shall just supply you with a good program to invert matrices as well as a good program to find all the eigen values of the matrix for the purpose of our class discussion I will just find that procedure to find the largest eigen value.

I will just outline steps to find the largest eigen value now let us look at this.

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## Eigenvalue of the largest magnitude

- Let A be a square matrix with n distinct eigenvalues such that $|\gamma_1| > |\gamma_2| > \cdots \ldots \ldots > |\gamma_n|$
- $\gamma_1, \gamma_2 \ldots \ldots \ldots . \gamma_n$ Eigenvalues

$$AV_i = \gamma V_i \qquad i = 1,2,\ldots\ldots N$$

$$\sum_{i=1,n} c_i V_i = 0 \quad \text{if and only if all } c_i = 0$$

$$\text{Let} \quad X_0 = C_1V_1 + C_2V_2 \ldots \ldots + C_nV_n$$

So if A is a square matrix it will have n distinct eigen values so suppose those n distinct values are such that I arranged them in a descending order that is lambda 1 which is my first eigen value suppose that is greater than lambda 2 which is greater than lambda 3 and which is greater than lambda n, so all these like lambdas are my eigen values so if such arrangement let us see how this strategy for finding the eigen values works.

As I mentioned already these eigen values are arranged in descending order so let me use the first eigen value equation Avi=lambda Vi. I going from 1 to n this is exactly the same as x earlier

I had AX=lambda X now I am saying Avi=gamma it should be gamma Ivi that is obvious gamma AVi which are all eigen values now all these Vi which are eigen vectors since I had n eigen values I will have these n eigen vectors.

And 1 of the theorems of vectors and matrices says that all these eigen vectors corresponding to different eigen values they are all linearly independent what is the meaning of linearly independent? If I have an equation like this i goes from 1 to n ciVi that = 0 only if all the ci are 0 so if the vectors are linearly dependent, then all the Ci will not be = 0 see for example take this vector i and j in 2 dimensions.

You know that in 2 dimensions I can write any vector has some Ai + Bj so any If I want to get Ai +Bj=0 the only way this can be 0 is both i and j both A and B are 0 if the co - efficient are not 0 I cannot get the sum off Ai + Vj=0 on the other hand suppose I take i and 2i this i and 2i are the vectors in the same direction let us say the x axis so if I have 2 vectors i and 2i they are not linearly independent because 1 is just the multiple of the other.

So, if I have 1 dimensions only 1 vector is linearly independent in 2 dimensions only 2 vectors are linearly independent and in three dimensions you know that i j k these are the three linearly independent vectors unit vectors. In this case they are not only linearly independent they are also orthogonal. So orthogonality is a very special case of linear independence. Linear independence is very general.

So, what I have done now AVi = lambda Vi and next since all the Vi are linearly independent so the other theorm states that any vector x in that dimension can be represented as a linear combination of all the eigen vectors. It is just like in three dimensions any vector in three dimensions can be represented as some of product some Ai+ Bj + Ck seek any vector in three dimension can be represented in some of these three ijk.

So similarly any vector in dimension can be written as a sum of product C1 V1 +C2 V2 +CnVn so these are my sum of these are the eigen vectors any vector is written as a sum of these vectors.
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Multiply $X_0$ successively (of course from the left side!) by $A, A^2 \ldots\ldots A^k$

- $AX_0 = C_1AV_1 + C_2AV_2 \ldots\ldots + C_nAV_n$

$$AX_0 = C_1\gamma_1V_1 + C_2\gamma_2V_2 \ldots\ldots + C_n\gamma_nV_n$$

$$A^2X_0 = C_1\gamma_1{}^2V_1 + C_2\gamma_2{}^2V_2 \ldots\ldots + C_n\gamma_n{}^nV_n$$

$$A^kX_0 = C_1\gamma_1{}^kV_1 + C_2\gamma_2{}^kV_2 \ldots\ldots + C_n\gamma_n{}^kV_n$$

$$= \gamma_1{}^k[\,C_1V_1 + C_2(\frac{\gamma_2}{\gamma_1})^kV_2 + \ldots\ldots + C_n(\frac{\gamma_n}{\gamma_1})^kV_n]$$

As 'k' becomes large all $\frac{\gamma_i}{\gamma_1}$ $(i = 2, \ldots, n)$ become small

So what I shall do now I shall multiply A* X0 so what is A* X0 what was X0? X0 was A1V1 A2V2 +AnVn so A* X0 will be C1AV1+C2AV2 and CnAVn so this is my AX0 when I multiply A square *A0 what is A square *A0 so first I got this gamma i V1 gamma i V2. How did I get gamma i V1 A *V1will give me gamma 1 V1 A*V2 will give me gamma2 V2 second eigen vextor second eigen value.

So, now I multiply A by the second time I get gamma 1 square V1 gamma 2 square V2 gamma n square Vn. So when I multiply k th times, so I will get C1 gamma k V1 C2 gamma k V2 and Cn gamma n k Vn. This n should actually be 2 here because it is A square, so I can now take this gamma 1 outside so gamma 1 ^ k C1V1 C2 gamma 2 gamma 1 k by dividing by this because I have taken gamma 1 to the k outside.

So when I multiply through gamma 2 to the k so now as k becomes large and since gamma 1 is the largest eigen value all these other terms will become smaller and smaller and go to 0 and only the first term will contribute that is what I have shown here now you see as k becomes very large only the first term will remain so my gamma 1 will be A k+1 X0 i * Ak X0i so that is how my gamma 1 will be calculated.

What is the strategy? Simple strategy multiply A many times that when I multiply k times only the first power first term will dominate all the others will go to 0 because gamma and by gamma

1 is very small because gamma 1 is the largest eigen value so that is my strategy. So, I will briefly summarize the strategy and we will actually use this in the program I am going to find an eigen value by taking powers of my matrix A multiplying on some vector X 0.

What is my X0 now? Let my X0 be 1 X20 X30 and so on this some eigen vector so I multiply A1 times this is what I got then what I do I multiply 2 times 3 times on these my algorithm so let me just summarize what is my final result?

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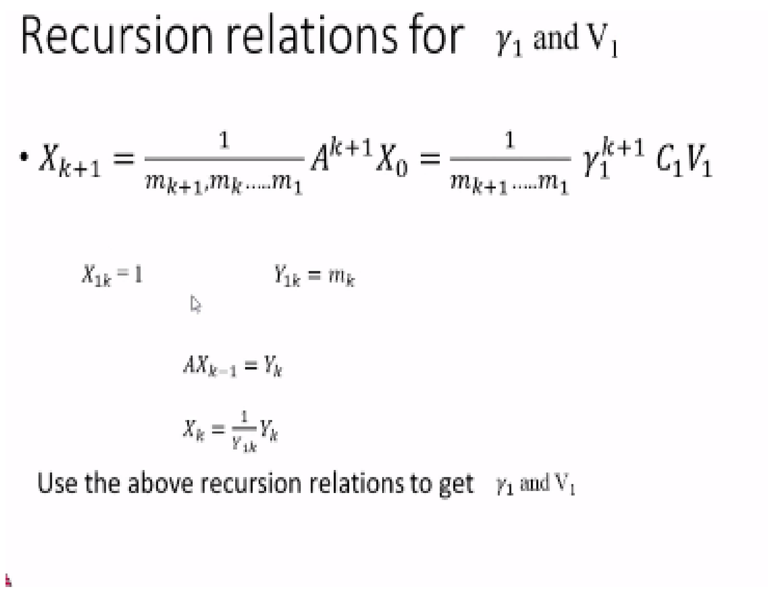


We will actually do the program in this A * Xk -1 is Yk and X k is 1 / Y 1k * Yk so basically, I get my gamma i and V1 by multiplying A repeated number of times so what I shall do. I shall keep each 1 slide so that you can see this.

**(Refer Slide Time: 29:17)**

## Calculating the largest eigenvalue and eigenvector

- $A^k X_0 = C_1 \gamma_1{}^k V_1$

$$A^{k+1} X_0 = C_1 \gamma_1{}^{k+1} V_1$$

$$\gamma_1 = (A^{k+1} X_0)_i / (A^k X_0)_i \qquad \forall\, i = 1, \ldots\ldots n$$

$Define\ a$ transposed "normalised vector" $as\ X_0{}^t = [1, X_{20}, X_{30}, \ldots X_{n0}]$

$$A^1 X_0 = AX_0 = Y_1 = m_1 X_1$$

$$\frac{1}{m_1} A^2 X_0 = AX_1 = Y_2 = m_2 X_2$$

Shown you for a sufficient time now let me go to the next slide.

**(Refer Slide Time: 29:20)**

## Calculating the largest eigenvalue and eigenvector

- $\frac{1}{m_1 m_2} A^3 X_0 = AX_2 = Y_3 = m_3 X_3$

$$\frac{1}{m_{k-1} \ldots\ldots m_1} A^k X_0 = AX_{k-1} = Y_k = m_k X_k$$

$$\frac{1}{m_k \ldots\ldots m_1} A^{k+1} X_0 = AX_k = Y_{k+1} = m_{k+1} X_{k+1}$$

$$Y_k{}^t = [Y_{1k}, Y_{2k}, \ldots\ldots Y_{nk}] \qquad X_k{}^t = [1, X_{2k}, X_{3k}, \ldots\ldots X_{nk}]$$

I shall display for sufficient time multiplying a many times I am taking out this mi below so just look at this slide I will show the next slide for some more time.

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## Calculating the largest eigenvalue and eigenvector

$$Y_{k+1} = \frac{1}{m_k \ldots\ldots m_1} A^{k+1} X_0 = \frac{1}{m_k \ldots\ldots m_1} \gamma_1^{k+1} C_1 V_1$$

$$X_k = \frac{1}{m_k \ldots\ldots m_1} A^k X_0 = \frac{1}{m_k \ldots\ldots m_1} \gamma_1^k C_1 V_1$$

$$\frac{Y_{1,k+1}}{X_{1,k+1}} = \frac{\frac{1}{m_k \ldots\ldots m_1} \gamma_1^{k+1} C_1 V_1}{\frac{1}{m_k \ldots\ldots m_1} \gamma_1^k C_1 V_1} = \gamma_1$$

$$X_{1,k+1} = 1 \qquad Y_{1,k+1} = \gamma_1$$

I have defined these Y k and Y k are 1/ mk up to m1 Ak +1 k0. It is gamma 1 to the k +1 C1 V1 and so finally I get X k now if X k it does not change anymore if X k does not change anymore that means I have a converse result.

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## Recursion relations for $\gamma_1$ and $V_1$

- $$X_{k+1} = \frac{1}{m_{k+1} m_k \ldots\ldots m_1} A^{k+1} X_0 = \frac{1}{m_{k+1} \ldots\ldots m_1} \gamma_1^{k+1} C_1 V_1$$

$$X_{1k} = 1 \qquad Y_{1k} = m_k$$

$$AX_{k-1} = Y_k$$

$$X_k = \frac{1}{Y_{1k}} Y_k$$

Use the above recursion relations to get $\gamma_1$ and $V_1$

If X k +1 is the same as Xk I have found the final result so what I shall do, we shall just execute this program fully so that you will know how to get the largest eigenvalue so in the next class what I will do I will consider the matrix inversion program as well as a matrix diagonalization program which diagonalize only the largest value which you get which we give using which we get the largest value to get all the values is not trivial.

So what we will do we will take an established program from some source and use it for our purpose but as far as our course is concerned you should know how to invert a matrix and you should know how to get the largest eigen value of the matrix and you should know all the concepts related to eigen values and eigen vectors I will conclude here. Thank you.