Advanced Mathematical Methods for Chemistry
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Module - 02
Lecture - 03
Rotational Matrices, Eigenvalues and Eigenvectors

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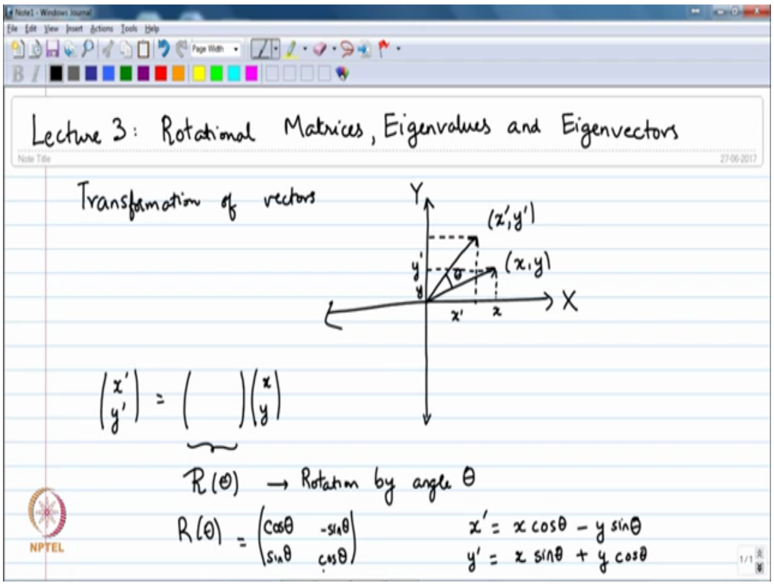

In today's lecture we are going to talk about Rotational matrices, Eigenvalues and Eigenvectors. So, so far we have already seen certain special kind of matrices, we saw orthogonal matrices and what we said is that orthogonal matrices they leave the length of a vector the same. So, now rotational matrices are again defined in terms of transformations of vectors.

So, we can ask the question what is the matrix that transforms a vector in the following way. So, suppose you have a vector I will just take, I will start with 2 dimensional space just to illustrate my point then you can go to 3D space or other spaces as required. Suppose you have a vector in 2 dimensional space that is represented by some arrow. So, this is my vector and let me call this vector x y and let us say I want to take this vector and rotate it by an angle theta. So, rotated by an angle theta and then I get some vector x prime y prime.

Now, so I can write this in the following form. So, I have a vector x prime y prime which is obtained from taking the vector x y and rotating it. So, the transformation, so you want a transformation that takes this vector x y to this vector x prime y prime and as we said before general linear transformation is represented by a matrix and, so this matrix this 2 dimensional matrix this 2 cross 2 matrix is what is called the rotational matrix and I will just call it R of theta. So, this is rotation by angle theta and you can easily see that R of theta has the following form it is a 2 by 2 matrix and you can easily work out by looking just by basic trigonometry you can work out that this is x prime, this is y prime, this is x this is y.

So, you can easily work out how x will be obtained from y, how x prime will be obtained from x and y and I will not work out the details, but this matrix has this form cos theta minus sin theta sin theta cos theta. So, this is the rotation matrix. So, and you know you know just to just to emphasize we had we got this from the expression x prime equal to x times cos theta minus y times sin theta and y prime is equal to x sin theta plus y times cosine of theta. You can easily work this out, it is not very difficult. Now and so we immediately we saw that the rotational matrix is given by this matrix.

Now, you would expect that since you are only rotating the vector you are not changing its magnitude and therefore, you expect that that R of theta should be orthogonal.

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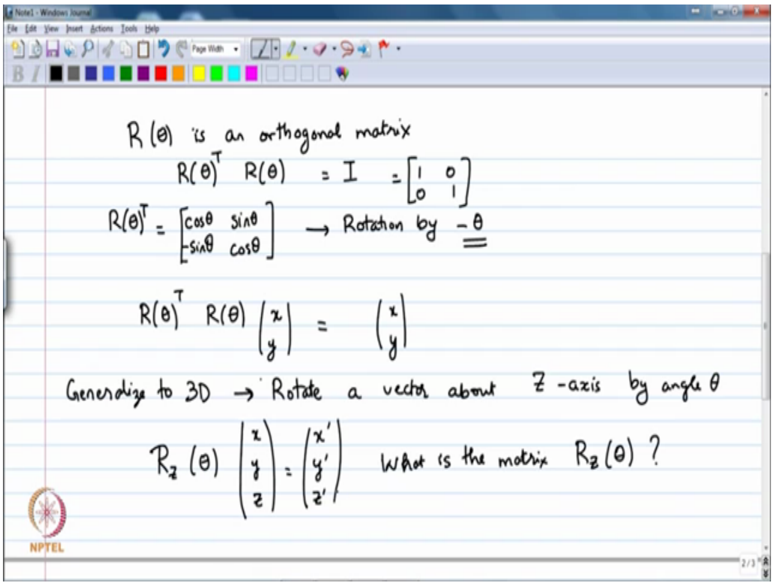

It is an orthogonal matrix and you would expect that R of theta transpose should be equal to R of theta inverse or in other words R of theta transpose times R of theta is the identity which is in this case it is given by 1 0 0 1 . So, now, what is R of theta transpose? So, R of theta transpose is basically you have cos theta and now you will have a, you will have a sin theta here you will have a minus sin theta here.

And you will have a cos theta and you can clearly see that this transpose is corresponds to rotation by minus theta. So, suppose you are rotating by minus theta then you can easily see that if you are rotating by minus theta then cos of minus theta is same as cos theta sin of minus sin minus theta will be plus sin theta this will be minus sin theta this will be cos theta. So, you can easily see that if you rotate by minus theta you will get such a matrix and you can clearly see that if you take a vector rotated by theta and then again rotated by minus theta you will get back the identity matrix. So, you will get back the original vector.

So, you can see in other words suppose I take, suppose I take R theta transpose R theta. So, first and I operated on this vector x y, this is equal to x y. So, clearly R is an orthogonal matrix this is called the matrix of rotations. Now in this operation when you did this rotation you can ask the question what is the axis about which we rotated. Now in this case we imagine that this axis is perpendicular to the plane of the paper and this and you are rotating by an angle theta about this axis. So, what this means is that if you had a vector in 3 dimensions. So, generalize to 3 dimensions now just imagine that you rotate by, rotate about z axis a vector about z axis by angle theta.

So, in other words you have you have something like x y z and you rotate by rotate about z axis by angle theta. So, now, what would be the rotate, what would be this matrix? So, what is the matrix R z of theta? So, now, you can you can easily see how to get this matrix.

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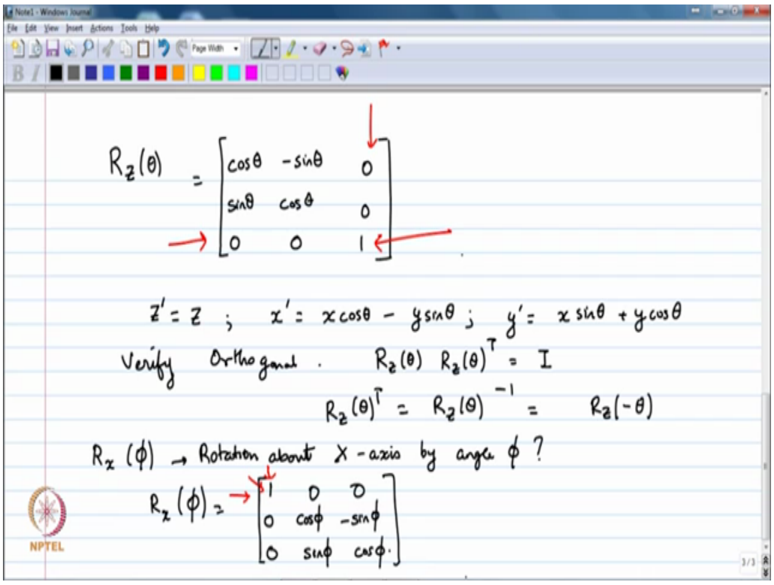

So, what we will do is we can; I will just write the expression for R z of theta and I will motivate the answer and you can easily verify this.

So, if you rotate any vector about the z axis by angle theta then the first thing is that if I take any then the z coordinate of the vector will be unchanged. So, since the z coordinate is unchanged. So, you can immediately see that z prime will be equal to z and just, this if we do not denote by x prime, y prime, z prime. So, clearly z prime has to be equal to z.

Now that implies that this part should be 0 0 1, 0 0 1, z prime has to be equal to z and x prime equal to x cosine theta minus y sin theta and y prime equal to x sin theta plus y cos theta. So, they are independent of x, of x and y and so this will just be the same rotational matrix, the same 2 by 2 rotational matrix that we had before that is R z of theta. So, R z of theta is this 3 cross 3 rotational matrix which has 0 0 1 and on along the third direction.

So, this corresponds to rotation around z by theta and there you can clearly verify that this is orthogonal very easy to see. So, verify orthogonal that is R z of theta, R z of theta transpose is nothing, but the identity. In other words R z of theta transpose equal to R z of theta inverse is equal to R z of minus theta. So, that is rotation by minus theta about z axis is same as inverse of rotation by about of z axis by theta and that is exactly equal to the transpose of this matrix of rotations.

So, these rotational matrices are extremely useful in lot of ways often we want to understand symmetries of molecules then we often use these rotational operations and now we have a general way to rotate any vector about in this case we have chosen the z axis. What about let us say if you want to rotate about the x axis by an angle phi. So, then in this case you can easily work out R x of phi will be given by, now in this case the x coordinate is the 1 that is unchanged. So, the x coordinate is the 1 that is not changing you will have instead of 0 0 1 in the case of R z you had the z coordinate that was not changing. So, you had a 1 here and these were these were 2 0s, now in this case you have the 1 here and these are 0s and the rest part will look very similar

So, now, instead of you will have a cos phi minus sin phi, a sin phi and a cosine phi and again you can verify that this is orthogonal and you can also verify that that it is the transpose is nothing, but its inverse you can also do rotation about the y axis and you can do rotations.

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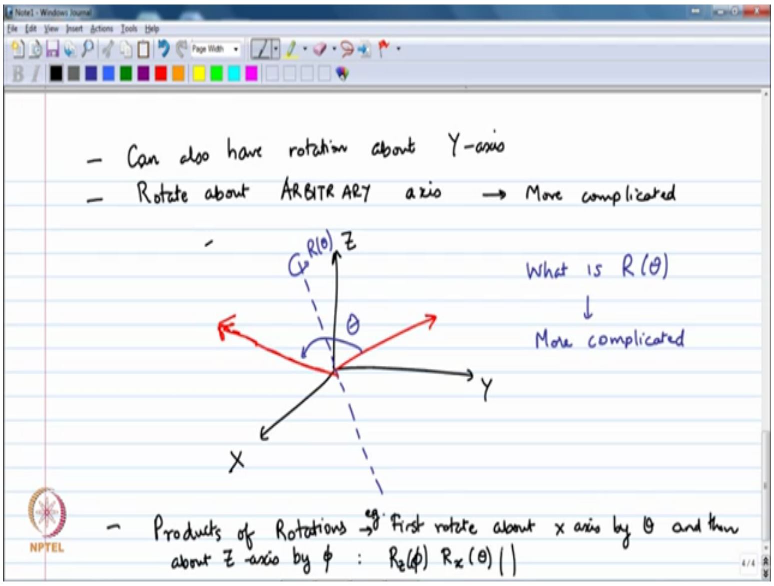

I will just write can also have rotation about y axis, I will also say some other things you can rotate about rotate about arbitrary axis this is more complicated.

So, in other words if you have your, if you have your coordinate system like this if this is x y z and you have some vector I will show it in red, if you have some vector like this and now if you imagine that you want to rotate this vector by some angle about some axis that could be something completely different there could be an axis like this and then we are really thinking in terms of 3 D. So, you could have an axis like this and you could rotate by angle by some angle theta about this axis. So, this vector is rotated and it ends up somewhere here.

So, then you could ask the question what is the matrix for this row. So, you are rotating by angle rotating about this axis by angle theta. So, what is (Refer Time: 15:03). Now this is a considerably more difficult question. So, so this is more complicated, but can be worked out and I want I will not detail the steps that you need to work it out, but you can definitely look up various books and see how to work this out. So, I just wanted to mention that these rotation matrices are quite useful you could also consider you could also consider things like products of rotations.

For example you could say first rotate about x axis by theta and then about z axis by phi. So, suppose you add something like that. So, the corresponding matrix would be given by would be given by something like this. So, first the first operation is by is by R x by theta then the next operation because your vector will come to the right of this. So, this is where your; this is where your vector will come. So, the next operation is by R z by phi. So, you will write it in this form you will write R z by phi times R x by theta.

So, all these are, all these are things that you can do with the rotational matrices and you know when we are doing the when we are doing the when we are doing the exercise we will see some examples of using these rotation matrices.

So, what does the rotational matrix do it takes a vector and it rotates it by some angle keeping the length fixed.

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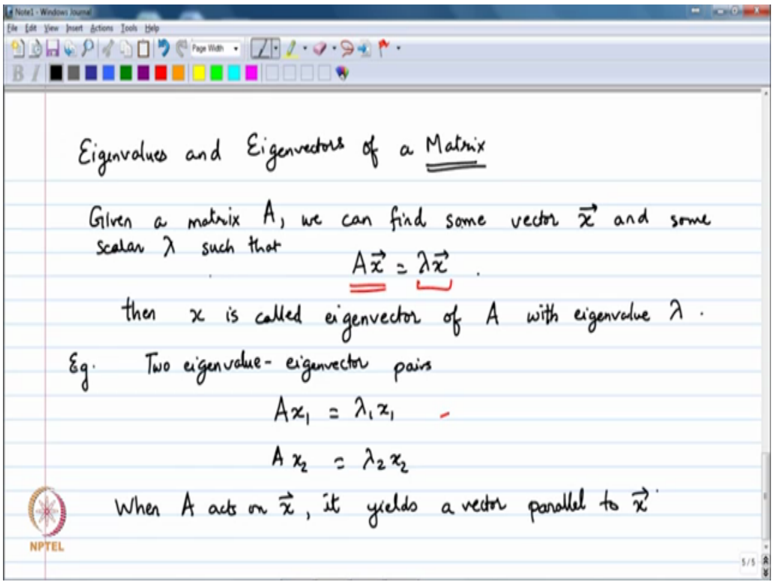

Now, the next concept that I want to talk about is that of eigenvalues and eigenvectors and let me emphasize this part of a matrix. And it is very important to understand that this idea of eigenvalues and eigenvectors is formulated based on the idea that you have you are given a matrix and you want to find its eigenvalues and eigenvectors.

So, let me write, given a matrix A we can find some vector x and some scalar lambda such that A x equal to lambda x and if we can do this then x is called eigenvector or let me let me put a vector arrow just to make sure that you do not confused and that you do not get confused with this eigenvector of A with eigenvalue lambda. So, this eigenvalue corresponds to this eigenvector and vice versa this eigenvector corresponds to this eigenvalue. So, if you have a different eigenvector you will have a different eigenvalue. So, you could have something like this, you could have a you could have a two eigenvalue eigenvector pairs.

So, for example, you could have something like A x 1 equal to lambda 1 x 1 and A x 2 equal to lambda 2 x 2. Notice for the same matrix A I have a pair of eigenvalues. So, example, this is nothing but an example, you could have 2, you could have 3, you could have 4, you could have as many as you could have different numbers.

So, now what is happening here? Let us think in terms of transformation. So, in terms of transformation what we are doing is A x is a transformation of a vector, it is a linear transformation of vector to give you another vector. So, what we are saying is that you are given a matrix A it takes a vector and gives you another vector. Now, given this matrix a you we are asking what is a possible vector which when operated by A just gives another vector in the same direction. So, the question is, the point is there. So, when A acts on x it yields a vector parallel to x. So, in other words it yields something in the same direction it does not change the direction of x. So, it yields a vector that is in the same direction as of x so, that is what is meant by an eigenvector and an eigenvalue. So, eigenvectors represents those directions which are preserved. Now; and some interesting things about eigenvectors.

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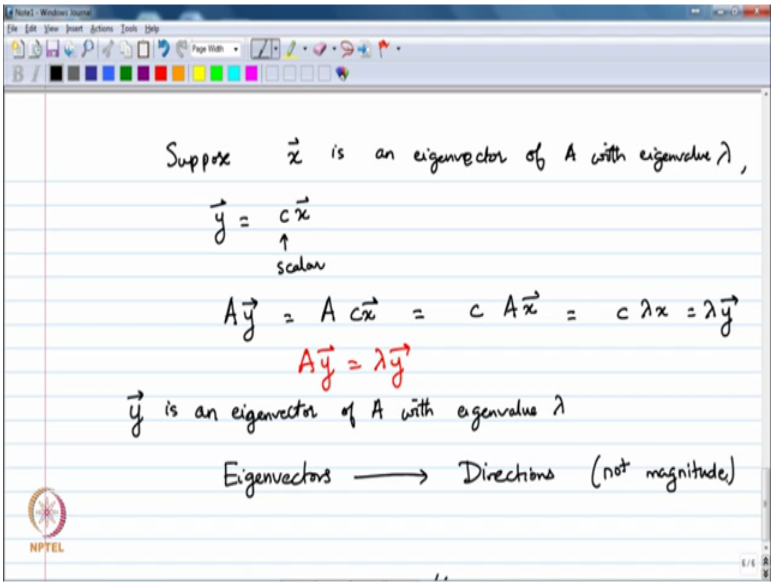

So, suppose x is an eigenvector of A with eigenvalue lambda it is important that each vector is connected with an eigenvalue or each eigenvalue is connected with an eigenvector. So, x is an eigenvector of matrix A which eigenvalue lambda.

Now, suppose I take c times x where c is a scalar, c is a scalar now c times x, let me say y is a vector that is c times x, c times x is another vector. Now you can clearly see that A times y is equal to A times c x is equal to c times A x c is just a scalar you can take it to the left. So, now, A x is lambda x. So, it is c times lambda x and this is I can switch the lambda and c and I can write this as lambda y.

So, in other words if you just look at this equation. So, so we get A y equal to lambda y. So, what this says is that y is an eigenvector of a with eigenvalue lambda. So, basically if you take an eigenvector multiplies by constant you will get another eigenvector with the same eigenvalue. So, that is why eigenvectors really refer to directions and not magnitudes, eigenvectors refer to directions not magnitudes because you can always multiply an eigenvector by a constant and get another eigenvector. So, when you talk about distinct eigenvectors we want eigenvectors pointing along different directions

Now, how do you determine eigenvalues and eigenvectors of a matrix? So, how will we determine the eigenvalues and eigenvectors of a matrix?

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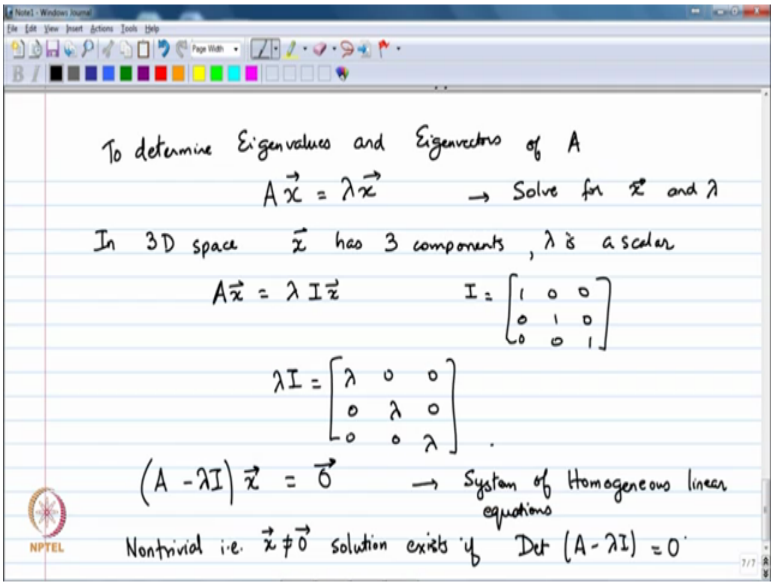

So, suppose you want to determine eigenvalues and eigenvectors of A, we have an equation A x equal to lambda x and you solve for x and lambda. So, with this one equation you want to solve for lambda and x. Now let us say in 3D space, x has 3 components and lambda is a scalar it looks like there are 4 unknowns and there are only 3 equations. So, A x equal to lambda x represents 3 equations it is a vector equation and since you are in 3D space you have 3 equations, but, so it is you have 3 equations and you have 4 things that you have to determine, so it appears like that, but as we will see eigenvectors only refer to directions and not magnitudes. So, we do not really need to worry about the magnitude. So, you can in fact, determine the directions the distinct direction. So, basically of these 3 components we can only determine 2 independently and one is 2 or 2 can be determined and 1 can be chosen independently.

Let us just let us try to work this out how will you go about doing this. So, now, A x equal to lambda x. So, what we will do is we can write this as A x equal to lambda times

I x where I is the identity matrix and lambda I. So, I is equal to 1 0 0, 0 1 0, 0 0 1 and lambda I is nothing, but lambda 0 0, 0 lambda 0, 0 0 lambda. So, then I can write a minus lambda I, so I take the lambda I to the left multiplied by x vector is equal to the 0 vector and this is a system of homogeneous of or sorry yeah; system of homogeneous linear equations.

So, this is a system of homogeneous linear equation and we already mentioned that the non trivial will that is x not equal to 0 solution exists if determinant of A minus lambda I equal to 0. So, we already saw when we were trying to in the problem set from the previous module we saw that when we wanted to look at linear independence of 3 vectors in 3 dimensional space we got the system of homogeneous linear equations and we said that the non trivial solution that is x naught equal to 0 solution exists only if this determinant is equal to 0.

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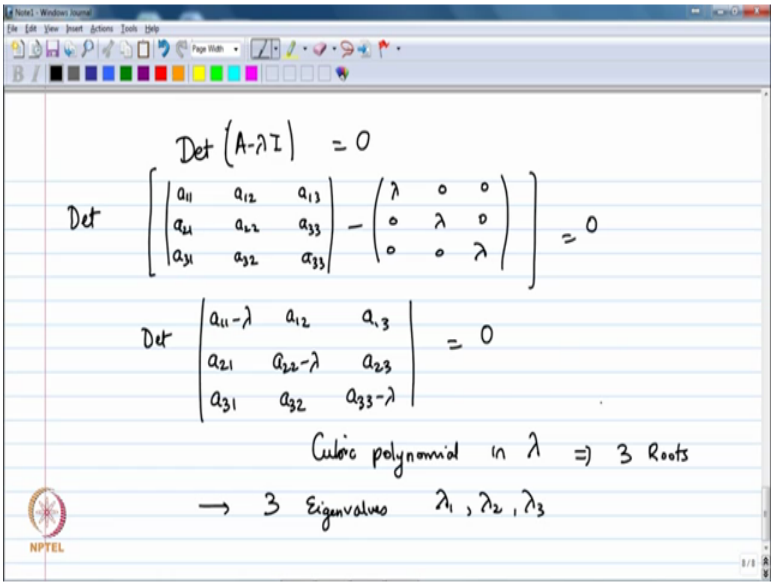

So, now, we have additional condition, and this will help us get your eigenvalue. So, the determinant of A minus lambda I equal to 0, now this, what will this look like? So, this will look like. So, this is the matrix a minus lambda I. So, if you write your usual your usual notation. So, you say a 11 has these components a 11, a 12, a 13, a 21 a 22, a 33, a 31, a 32, a 33. Now if you subtract lambda I. So, you have this minus lambda I is lambda 0 0 0 lambda 0 0 0 lambda. So, this is A minus lambda I and you have the determinant of this equal to 0.

So, what this look like, this is this look like determinant of a 11 minus lambda a 12 a 13, a 21 a 22 minus lambda a 23, a 31 a 32 a 33 minus lambda this determinant equal to 0, the determinant of this is equal to 0. And you can clearly see that when you take the determinant you will get this if you just look at the diagonal term you will have a term that involves lambda cube. So, this is a cubic polynomial in lambda. So, the left hand side is a cubic polynomial in lambda and, so that implies that there are 3 roots.

So, we have a cubic polynomial lambda equal to 0. So, you have 3 roots, so basically you can determine 3 eigenvalues lambda 1, lambda 2, lambda 3, I will just call them lambda 1, lambda 2, lambda 3. So, you can determine 3 eigenvalues for this equation and you can take each eigenvalue so corresponding to lambda 1 to each eigenvalue value we can determine corresponding eigenvector.

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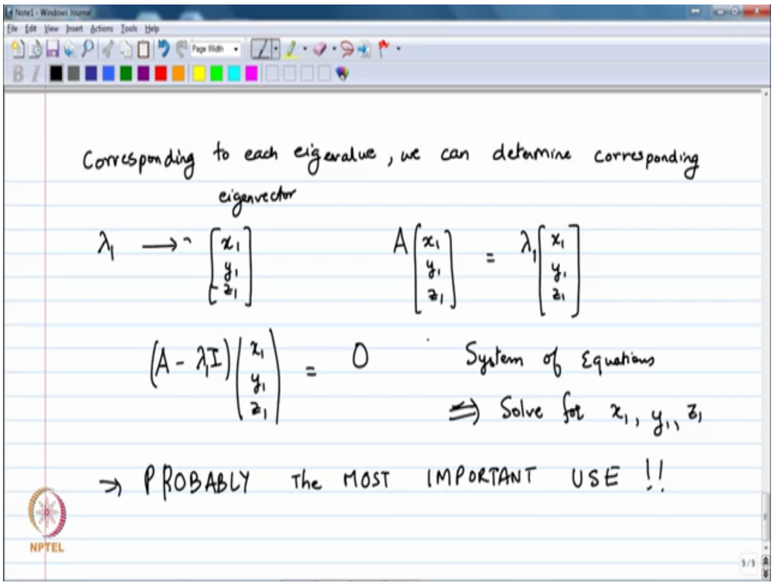

So, for example, for example, if you have lambda 1 we write the corresponding eigenvector as x 1, y 1, z 1. So, if you write the eigenvector in this form eigenvector these are the components of the eigenvector then you can clearly show that since you have A times x 1, y 1, z 1 is equal to lambda times x 1, y 1, z 1 then what you have is you have the equation A minus lambda I times x 1, y 1, z 1 of A minus lambda 1, algebra lambda 1 is equal to 0 and this is a system of equations and you can solve for x 1, y 1, z 1.

And since this is a homogeneous equation you can only determine 2 of them independently the third one you can or 2 of them you can determine if you fix the third one and we will see examples of this as we go. But the point is now we know how to calculate eigenvalues and eigenvectors of a matrix and this is probably the most I emphasizes, so this is probably the most important use of matrices, important concept or most important I will rather I will say in terms of utilization. So, this is the probably the most important use of matrices.

So, I will stop today's lecture here and just to remind ourselves we first learnt about rotational matrices and then we learnt about eigenvalues and eigenvectors.

Thank you.