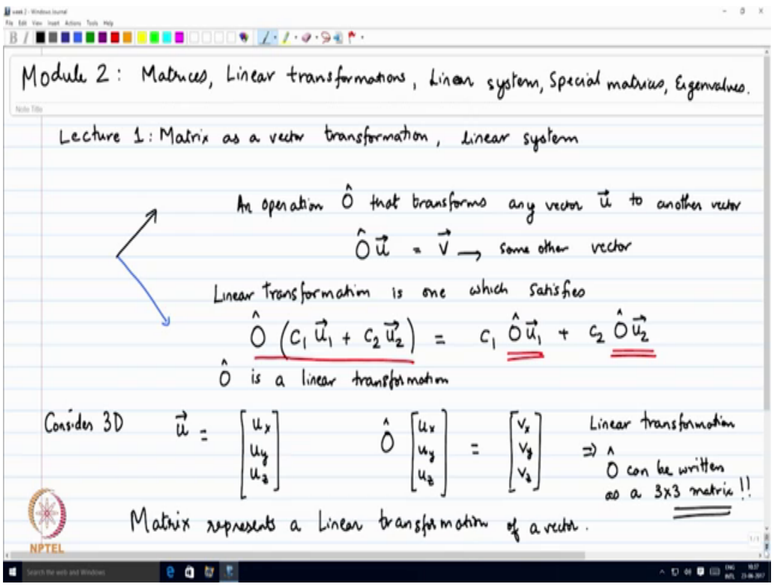
Advanced Mathematical Methods for Chemistry

Prof. Madhav Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Module - 02
Lecture - 01
Matrix as a Vector Transformation, Linear System

Now we will start module 2 and in this module I will be dealing with matrices mainly we look at what are called as linear transformations, we look at a linear system of equations and we will look at some special matrices then we will discuss eigenvalues we will also talk about matrix inverse.

(Refer Slide Time: 00:24)



So, I will start this with the first lecture where we will be looking at the matrix as a transformation of a vector. Let us to give you an idea of how matrices appear naturally let us think of the following. Imagine that you have some vector and I will just show it by some arrow and just showing 1 vector and let this be in 3 dimensional spaces. So, now, you can transform this vector imagine that you do some operation, and after the operation you get a new vector which is shown let us say by this. So, what you have done you might have changed both the magnitude and the direction of the vector. So, you transformed it and you got a new vector.

Now, imagine that you do this to all the vectors in the vector space, if you imagine an operation that takes an operation that transforms all the vectors in the vector space. O I will put a hat on it transforms any vector u to another vector.

Student: Of.

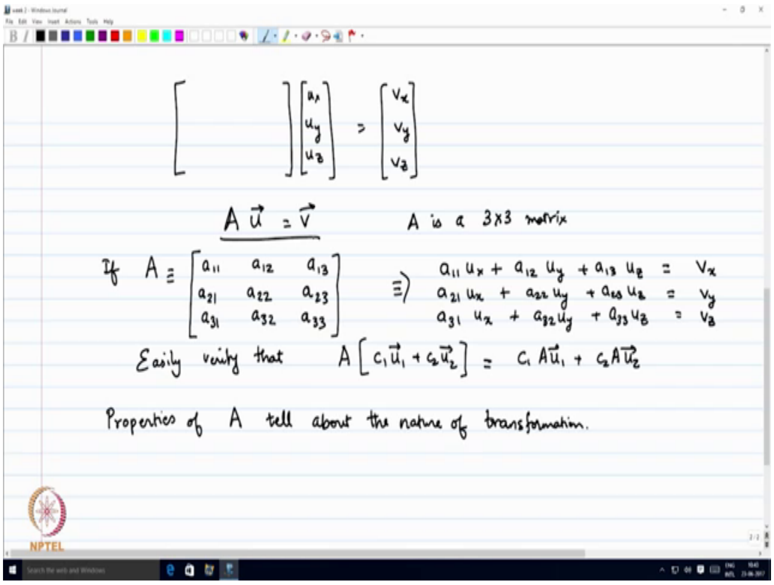
For example this operate this operation O my transform u, to give you some vector v some other vector. So, this is some other vector you could imagine that you can do the same thing on all vectors and you will get various other vectors. Suppose you have a transformation a linear transformation is 1 which satisfies the following.

So, suppose you had C 1 u1, u 1 is 1 vector C 1 is an arbitrary constant plus C 2 u 2 when this operate when this transformation acts on this vector. So, if u 1 is a vector u 2 is a vector then C 1 u 1 plus C 2 u 2 is also a vector, and when this operation acts on this vector u its effect can be written as C 1 times the operation on u 1 plus C 2 times the operation on u 2. So, this is called a linear transformation because what its see also operation on u 1 will give you another vector, operation on u 2 will give you another vector. So, C 1 times this vector plus C 2 times this vector will give you another vector. The operation on the on a linear combination of vectors can be written as a linear combination of operations; any operation that satisfies this is called so, O is a linear transformation.

You can think what the linear transformation will look like let us consider 3D. So, my vector let me write u in terms of its components I will write it as a column vector. So, I will write it as u x, u y, u z. So, I am writing it as a column matrix. Now what you have is operator O which is for acting on u x, u y, u z to give you something else some other vector and that vector I also write it as a column matrix and I will write it as v x v y, v z. So, I can do any operation can be represented by this way, but linear transformation implies O can be written as a 3 by 3 matrix. So, if this is a linear transformation then I can write this O as a 3 by 3 matrix, because if I take a 3 by 3 matrix and I multiply 3 cross 1 column then I will get another vector.

So, I will get another 3 cross 1 vector the most general. So, a matrix represents a linear transformation of a vector and you can easily show that if you have a matrix operating on this linear combination you can easily show that your matrix will satisfy this. So, a matrix operating on a linear combination of vectors can be written as a linear combination of matrix operating on the individual vectors.

(Refer Slide Time: 05:35)



This is the most important idea of matrices. So, matrix represents a linear transformation of a vector, we will write this in the form that you are more familiar with. So, what you will say is that if you have a matrix multiplied by a vector you will get some other vector this is a 3 by 3 matrix, we will often write this in the following form. So, if you can write this as A times u equal to v where A is A 3 cross 3 matrix, we just investigate this a little more deeply. So, why we said this is a linear transformation.

Now, notice this equation I can write in the following form o. So, if A is given by this matrix this is a very typical notation that is used for matrices for matrix elements. So, those are the elements of A are often written in this form, 1, 1, 1 2, 1, 3, 2, 1, 2, 2, 2, 3, 3, 1, 3, 2, 3, 3. So, there is an easy way to describe the elements of a matrix using this notation. So, if a had this form then we can see this a u equal to v is actually written in this form. So, a 11 u x, plus a 1 2 u y plus a 1 3 u z is equal to v x, a 2 1 u x, plus a 2 2 u y plus a 2 3 u z equal to v y and a 3 1 u x plus a 3 2 u y plus a 3 three u z equal to v z.

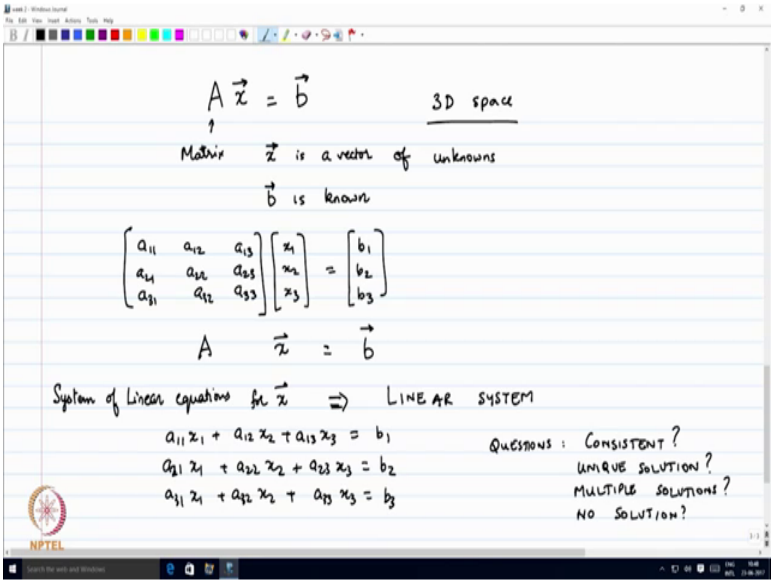
So, this this equation a u equal to v actually corresponds to these 3 equations, and now and now you can see where the phrase linear transformation comes. See what we did is we are writing v x as some function of u x, u y, u z, but notice that function does not involve any squares of u any products of us it just has u x multiplied by a constant, u y multiplied by a constant, and u z multiplied by a constant and addition of them. It does not have any u x square, it does not have any u x u y term. So, all the terms are proportional to u x or u y or u z. So, there are no products. So, that is why it is a linear combination of u x, u y and u z.

Similarly, v y is a linear combination of u x, u y, u z, v z is a linear combination of u x u y u z. So, therefore, these transformations are referred to as linear transformations and you can easily verify that A operated on I will just write C 1 u 1, plus C 2 u 2 is equal to C 1 a u 1 plus C 2 a u 2. In other words this A matrix can be thought of in terms of a linear transformation of a vector. So, it takes a vector gives you another vector and it is a linear transformation you can also have non-linear transformation of vectors, but this is a linear transformation. This idea of matrices is extremely useful because now you can ask questions like what kind of transformations can have suppose I look at all vectors then what does this transformation do to all vectors, and later on you will see some very specific kinds of transformation of soft vectors and those specific kinds of transformations will be represented by specific matrices.

For example if the operation of this matrix on a vector is to rotate the vector by some angle, rotate every vector operation on any vector is to rotated by some angle then we will see that the matrix should satisfy certain properties and we will see something is called rotation matrices. But the point is that understanding properties of A tell about the nature of transformation to we will see that in a bit for example, you could have a transformation we just takes a vector gives the direction the same, but just stretches it out. So, what will what then what will your matrix a look like and so on.

Now, the other thing that I want to mention is this idea of is again seen in this expression A u equal to b.

(Refer Slide Time: 10:07)



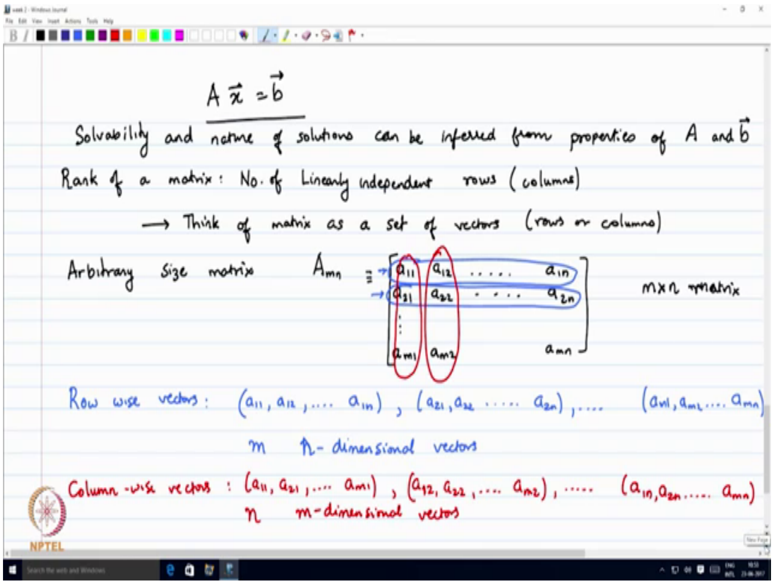
And this is the idea of a system of equations suppose you take A times u equal to or let me use a more standard notation. So, A times x x is a vector equal to b; now x is a vector. So, x is this vector that has 3 components and b is another vector with 3 components. So, let us for simplicity let us consider a 3 D space, but you can you can consider this for any arbitrary dimensional space.

So, A is a matrix. So, x is a vector of unknowns the variable x is used just to show that this is a vector of unknowns. So, b is known. So, then what you have is if you have this matrix. So, I can write this. So, if I write a 11 a 12. So, I am writing a in this form. So, this is my A x let me write it as x 1, x 2, x 3 is my x. So, this is A x and let me write b as b 1, b 2, b 3.

So, if all these a s are known and all the b s are known then you can solve for x. So, this is a system of linear equations for x and this is referred to as a linear system and what are the equations. So, the 3 equations for x 1, x 2, x 3 are a 11, x 1 plus a 12 x 2 plus a 13 x 3 equal to b 1 a 11 a 21 x 1 plus a 22 x 2, plus a 23 x 3 equal to b 2, a 31 x 1 plus a 32 x 2 plus a 33 x 3 equal to b 3.

So, clearly you have 3 equations to solve for x 1, x 2, x 3 this is a linear system of equations and so, you can see that matrices appear naturally in this linear system of equations and this is another very important application of matrices you will use matrices very often when you are writing this linear system of equations. So, now, one of the when you have these 3 equations and 3 unknowns or if you have any number of equations and any number of unknowns then you can ask are these equations consistent. So, the questions that come up or consistent is there a unique solution or there multiple solutions or is it no solution. So, these are some of the questions that come up and all these can be answered just by looking at the matrix and this vector b.

(Refer Slide Time: 13:20)



So, this linear system of equations where A x equal to b solvability of this and nature of solutions can be inferred from properties of A of matrix A and b. You need to know both the properties of A and vector b. Now I will just mention very briefly you may be familiar with this, but you can always read this up. So, this is there is a concept called the rank of a matrix. So, it is the number of linearly independent rows or you can look or you can say columns. So, what this means.

So, in order to describe the rank of a matrix you think of matrix as a set of vectors either in terms of rows or columns rows or columns. So, you think of this matrix as a set of vectors. So, I mean we thought of matrix as a transformation you could also think of this matrix. So, suppose you have and now let us take a arbitrary size matrix and this is A m n. So, here what is done is that you have a 11, a 12 all the way up to a 1n, a 21, a 22, a 2n and you go down all the way up to a m1.

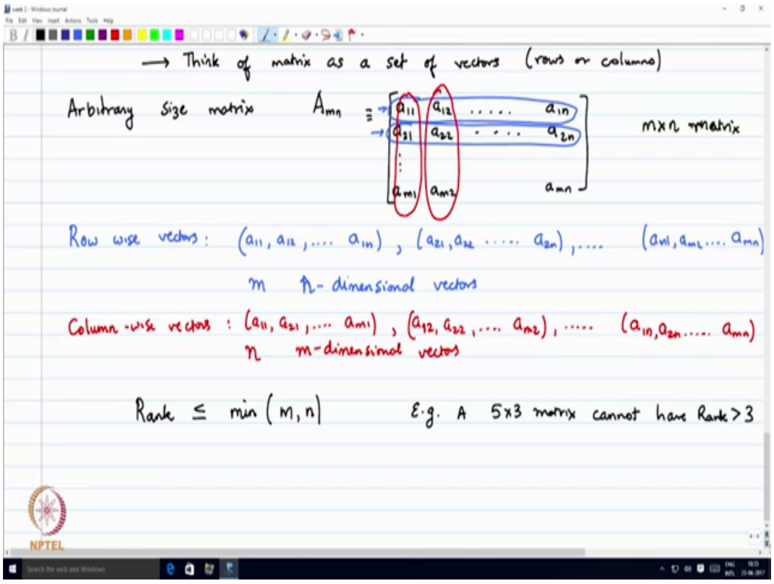
So, this is a m cross n matrix this is called an m cross n matrix. So, the rows number of rows and columns is not the same in this case. So, if you take an arbitrary size matrix and now you think of this matrix as a set of vectors. So, you can think of for example, you can think of vectors like this. So, this can be a vector this can be a vector. So, you think of vectors like row wise vectors or you can think of them column wise or you can think of or you can think of vectors in this direction this can be a vector this can be a vector ok.

So, what you do is. So, let us say you are doing it row wise vectors. So, that will be the first vector will be a 11, a 12, a 1n this is an n dimensional vector this is one vector, the second vector will be a 21, a 22, a 2n and you go on and on, so a m1, a m2, a mn. So, you have m you have a total number of m nn dimensional vectors. So, then you can ask how many of these are linearly independent or are these vectors linearly independent or not.

So, the number of linearly independent vectors; number of vectors that are linearly independent is called the rank is also alternatively if you are done using column. So, the first 1 I will write as a 11, a 21, a m1, a 12, a 22, a m2 all the way up to a 1n, a 2n, a mn. So, now, in this case you have n m dimensional vectors. So, these are m dimensional because each vector has m components here the each vector had n components.

So, you can do it either ways to calculate the rank of the matrix you can use either rows or columns and you can see how many of these vectors are linearly independent. So, how many of the vectors are linearly independent what; that means is that clearly the number of linearly independent vectors if you have n m dimensional vectors you cannot have more than more than n of them be linearly independent.

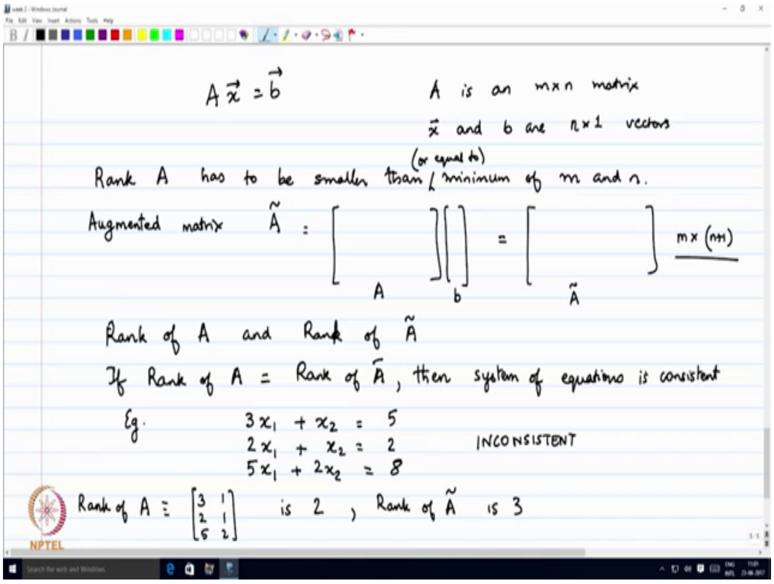
(Refer Slide Time: 17:26)



Similarly you cannot have more than m of them independent linearly independent. So, basically your rank is less than or equal to minimum of m and n.

So, your rank of the matrix cannot be greater than the number of linearly independent rows or columns. So, it has to be less than or equal to the minimum of m or n, whichever is smaller. So, if you have a 5 by 3 matrix your rank cannot be greater than 3. So, for example, 5 by 3 matrix cannot have rank greater than 3; now this concept of rank of a matrix is very useful to determine whether the solutions are possible and whether they are consistent or not I will just do that and this will be the last thing that I will mention here.

(Refer Slide Time: 18:19)



So, suppose you have A x equal to b, and let us say A is an m cross n matrix x and b are m cross O or n cross 1 vectors; that means, n dimensional vectors. So, they are written as column matrices. So, this it looks as an n cross 1 column matrix should be an n. Now if you have this case you know that the rank of a now rank of has to be smaller than minimum of m and n then the basically the smaller of the 2 numbers it has to be smaller than that smaller than or equal to. I should not say smaller than or equal to or equal to.

So, now what we have. So, what is the rank tell you. So, let us make another matrix. So, call the augmented matrix A tilde and this is given by. So, in order to write down the augmented matrix you write A here and you write b here and you make this matrix. So, the size of this matrix is A tilde. So, you just add this extra column. So, it is m cross n plus 1. So, it is an m cross it is an m times m n plus 1 matrix. So, it has m rows and n plus 1 column. So, this this augmented matrix what is done is you calculate rank of A and rank of A tilde, if rank of a equal to rank of A tilde then equations are consistent then the system of equations is consistent.

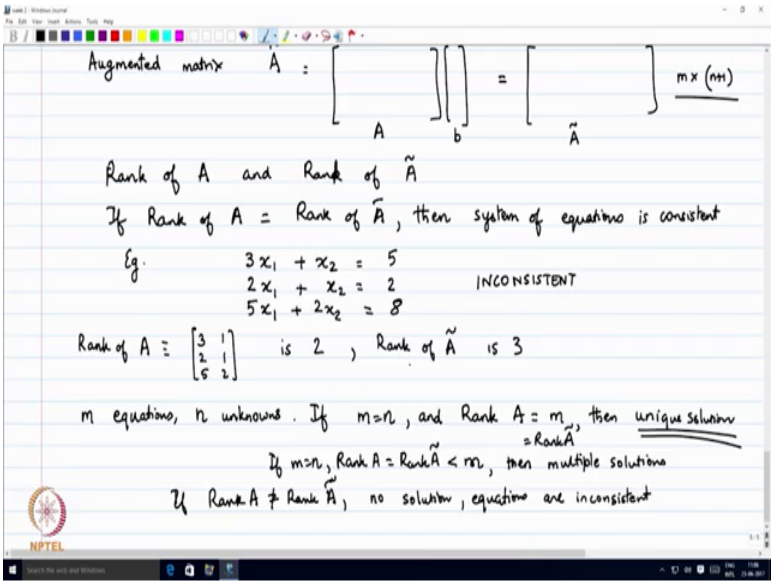
What do you mean by consistent set of equations? So, that means, there I mean I will just give an example of a set of equations that are not consistent. So, example if you say let us say you take 3 x 1 plus x 2 equal to 5 and let us say you take another set that says let us say 2 x 1 plus x 2 equal to 2 and you take a third equation. So, you have 2 equations now suppose you have a third equation that had let us say 5x 1 plus 2 x 2 equal to 8.

So, now suppose I had 3 equations and I had let us say I had just 2 unknowns; now what you can see is that the third equation is just a sum of the first two, but on the. So, the left hand side you had 3 plus 2 equal to 5 and 1 plus 1 equal to 2, so 5. So, it is just left hand side you just added up these 2 right hand side So, these are clearly not consistent and you cannot find any solution to this set of equations. So, this is an example of a system of equations that are not consistent and you know I took 2 equations and 2 unknowns, but I could do the same with 2 equations and 3 unknowns also or 3 equations and 3 unknowns I could do with an arbitrary number equations and unknowns.

But what you the point we want to make is that if you have taken this and you had calculated the rank of A. So, now, rank of A is equal to. So, what is my A matrix? So, A matrix is 3 1 2 1 5 2. So, rank of A is given by this is. So, if you just look at the rank of this matrix you can see that the third vector is the linear combination of these 2 is 2 and rank of A tilde is 3 you can easily verify this, you can easily verify this if you take A tilde then you will find that those 3 vectors are linearly independent. So, the rank of A tilde is 3. So, the rank is used to tell whether a set of equations are consistent or not ok.

So, now we have we can say whether the equations are consistent or not now further say m less than n.

(Refer Slide Time: 23:05)



Say I will just take a case where m is less than n. So, now if you if you see this. So, n is the or so, here you have m equations n unknowns.

So, if m equal to n and rank of A equal to m, then unique solution exists then the equations have a unique solution. So, that means, if all your m equations are linearly independent then there is a unique solution rank of A equal to rank of A tilde I should mention. So, this should be equal to rank of A tilde and you can look at the other conditions. So, if you have more equations and less unknowns. So, for example, let us take the case if m equal to n rank of A equal to rank of A tilde less than m then basically you get multiple solutions and you know what it means is you can choose some of the variables some of the unknowns can be chosen arbitrarily and the remaining are expressed in terms of those unknowns.

So, I do not want to go too much into this, but basically I want to mention that matrices they correspond to they can represent system of equations and matrices are involved in the system of equations, and you knowing the rank of the matrix can tell you what are the properties of this system of equations whether you have multiple solutions and or you have only one solution or one unique solution and you know as I said if rank of A naught equal to rank of A tilde, then no unique solutions no solution or equations inconsistent.

So, if you have. So, you can either have if of course, if you have more equations than unknowns then they better be consistent if we are consistent you can still get the solution, but if you have less equations and unknowns then you can find multiple solutions. So, this is the idea of matrix rank and you can see how this is helped us identify the properties of the solutions.

Now, I will stop here for this lecture. So, in the next lecture we will start looking at special matrices and we will see again we will get back to the idea may of a matrix as a transformation of a vector and look at certain special matrices.