Advanced Mathematical Methods for Chemistry

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Module - 01
Lecture - 01
Vectors, Vector Spaces, Linear Independence, Basis

Welcome to this course titled advanced mathematical methods in chemistry. This is going to be a 12 week course, and today we will start with the first week.

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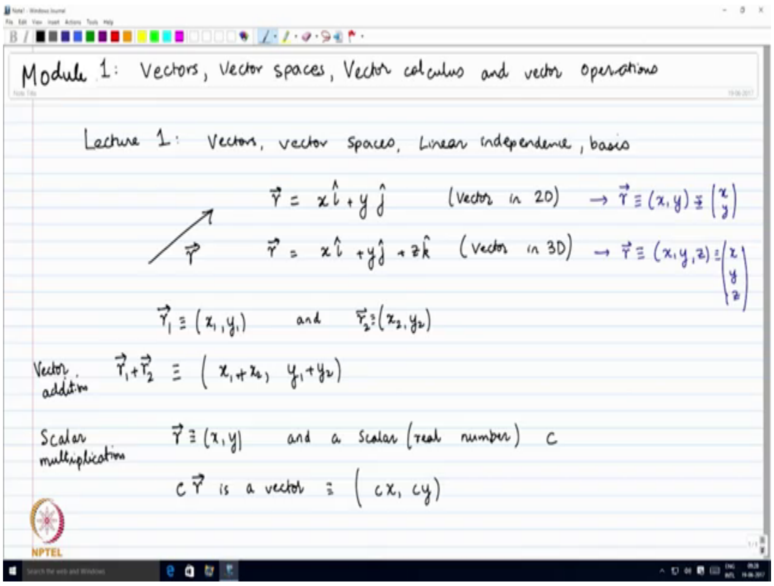

And the topics that we are going to discuss in this week are relay related to vectors vector spaces, vector operations and vector calculus. Today I will start talking about vectors vector spaces the idea of linear independence and basis vectors. So, all of you are familiar with vectors in some form. You might have heard of vectors as quant objects that have both a magnitude and a direction. So, for example, you could have a vector that is shown by an arrow in space. So, it has both a length which represents the magnitude and a direction which is represented by the direction of the arrow.

Now, this vector if you denote this vector by the notation r, and you would write a vector on top, then there are different ways in which you can represent this vector. For example, I could write r and assuming that this in a 2 dimensional space, I could write it as x times

I plus y times j. This is a vector 2 dimensions or you could have a vector in 3 dimensions which you might write in this form x I plus y j plus z k this is a vector in 3 D.

So, these are examples of how you write vectors. Now you could write this equivalently you could just write this in a in a different notation, for example, this you could write as you could write as just instead of this r vector, you could write it as x times y, x comma y which is a way of writing which instead of writing this I and j every time you just write it as x comma y. So, x and y are called the components of the vector x is the x component y is the y component of this vector r. Similarly, in 3D you might write r. So, it is of 10 denoted as x y z, where x y and z are the components of this vector. So, you do not have to explicitly write this i j and k. In some cases, we will also use a notation where this is represented as a equivalently represented lies the column vector. So, this might be written as x y or as a column matrix. So, this is a matrix representation of the vector.

So, the same vector can be written in different notations. So, you can write it as in this I j k notation or you can write it is in x comma, y comma z, or you can write as a column matrix. So, all these are notations for vectors, and in various cases you would be using one notation or the other as convenient. Now the nice thing about writing vectors in these forms is that you can immediately see how to add vectors. So, suppose you had one vector, I will do it, I will show it in 2 dimensional space suppose you had a vector r 1 which had components x 1 and y 1 and you had a vector r 2 which had components x 2 and y 2. Then you can have a vector r 1 plus r 2 which is a vector addition and this vector addition will yield a vector with 2 components x 1 plus x 2 and y 1 plus y 2.

So, what you do when you add vectors is to add them component wise, and similarly I can do this in 3 3 dimensions also I would not show this explicitly, but vector addition is something that you can easily do especially using this notation, another important operation on vectors is called scalar multiplication, where you take a vector for example, you could take a vector r, which is denoted by x y and a scalar a scalar is nothing, but a real number, and let me call the scalar c. So, if you had a scalar c and a vector r then you could construct you could multiply c times r, which gives you another vector. So, this is a vector and what are the components of this vector the components of this vector are c x and c y.

So, these are very these operations which are namely vector addition and scalar multiplication are extremely easy to do in this notation. And in fact, vect these are 2 operations that actually end up defining vectors. So, vectors are defined on the basis of these operations.

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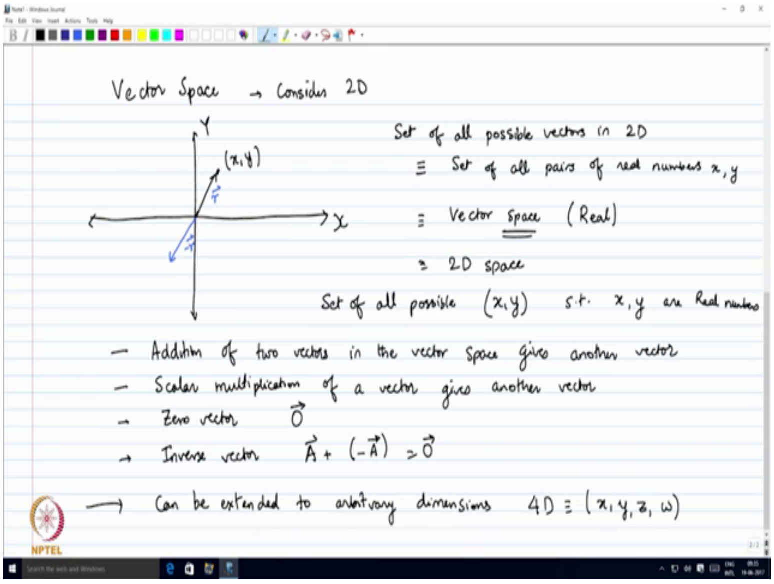

And we will see that in a minute, we will look at the idea of what is called the vector space. Vector space and to motivate this idea let us consider let us consider 2D first 2 D. So, now, in 2D you show a vector by an arrow. So, let me show the entire x y plane. This is the entire 2D space 2D coordinate space and this entire space of all coordinates will be related to what is called the vector space.

So, how do we understand what this vector spaces now if you take any vector in this 2D any vector can be represented by an arrow or it can be represented by a point x y the coordinates of that point are x y. So, now, suppose you take suppose you take the set of all vectors all possible vectors in 2D. So, this is basically equivalent to the set of all pairs of real numbers x and y. So, you take any 2 real numbers x y that that can represent a vector and the set of all pairs of real numbers represents the set of all possible vectors. And this is a vector space vector space the word space is used to denote this entire set. So, the set of all possible vectors is called the vector space and this is the usual 2D space.

Similarly, we can have a similarly we can do in 3D also. So, if you say what is 2D 2D 2D space or 2D vector space, this is the set of all possible all possible x y such that x and y are real numbers and this constitutes a vector space and in particular it is a real vector space. So, it is a real vector space because we insisted that x and y should be real numbers.

So, the set of all possible vectors in 2D constitutes a real vector space and this is a 2D dimensional real vector space, now there are some characteristics of this vector space that basically it does go back to the 2 operations that we talked about last time. So, addition of 2 vectors, in the vector space gives another vector. So if you add any 2 vectors you get another vector which is also in the vector space. Similarly, scalar multiplication of a vector, you can take a vector and multiply by any scalar and you will get another vector gives another vector these are easy to see because you can just take any vector multiplied by a scalar you will get a different vector and so that vector will also be in the same space.

So, this is the main characteristic of the vector space that you can add any 2 vectors or you can multiply by a scalar and you get another vector. So, and there are certain other fairly obvious things like there is something called as a 0 vector, 0 and there is something called an inverse vector. So, a plus any vector a plus a vector minus a gives you 0. So, the minus a is called the inverse of a additive inverse. So, these are certain and these are very obvious I mean for suppose you have suppose you look at this vector this vector that is shown here then you can you can you can you can easily see that an inverse for this vector would look something like this. So, if this is r then this will be minus r it is just the negative of that. So, that is the additive inverse such that you add up these 2 and you get the 0 vector.

So these are things that are also vectors. So, so the condition for something to be a vector space is that you take the collection of all possible vectors such that you add any 2 vectors you get another vector which is also in the vector space and n the vector space has a 0 vector, because I added a and minus a and I got a 0 which is his should emphasize this is a 0 vector. So, 0 vector is also a vector in the in the space and also there is an inverse additive inverse for every vector. So, these are the basic axioms which define something called the vector space. And the advantage of defining something like a vector space is that you can now extend this to any dimensions, you can go to 2D you can go to 3D, but you do not need to stop there you can go to 4D you can go to can be extended to arbitrary dimensions.

So, we have seen 2 ds we have seen 3D. So, for example, if you want 4D, 4D you can just write x y z w we can just have 4 variables. So, a collection of 4 numbers 4 scalars would form a 4D vector space. So, this is of this turns out to be fairly useful and it has lot of applications as we will see. Now we can will we will come to a, we will come to a formal definition of what we mean by the dimensionality in a in a few minutes, but before that we will introduce the idea of linear independence.

So, the next idea is the idea of linear independence of vectors. So, what does linear independence means?

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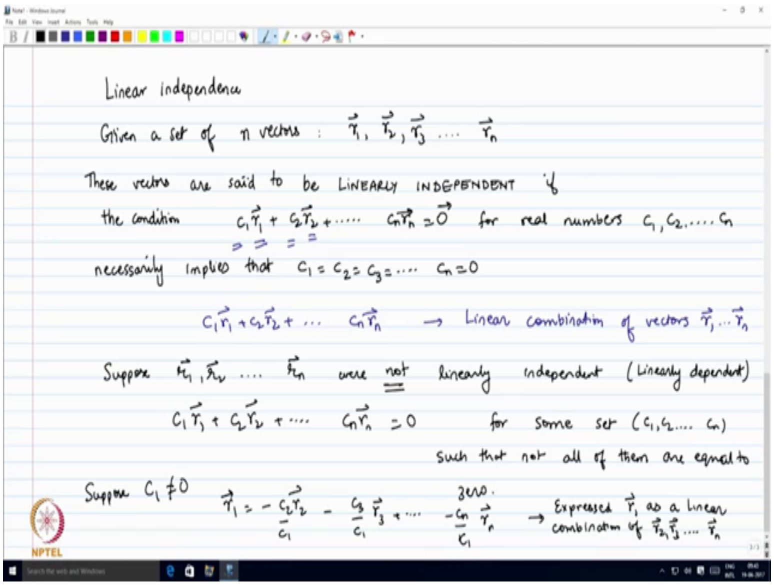

So, suppose you have a set of vectors. So, suppose I will just take for example, I will just take given a set of n vectors, I will denote them by r 1, r 2, r 3 up to r n. I am not saying anything about the dimensionality of the space or anything these are just n vectors in some vector space. So, if you are given a set of n vectors then you can ask are these linearly independent.

So, these vectors are said to be linearly independent. If the condition c 1 r 1 plus c 2 r 2 plus and so on up to c n r n equal to 0. So, for real numbers c 1 c 2 up to c n, if this condition implies that c 1 equal to c 2 equal to c 3 equal to up to c n equal to 0. So, if this condition necessarily implies that c 1 equal to c 2 and so on equal to 0, then the vectors r 1 up to r n are said to be linearly independent.

So, now few a few things I should mention. So, what we did here we multiply it by a scalar c 1. And then we took vector r 2 multiplied it by another scalar c 2, and we added up these 2 vectors, similarly we did that for all the remaining vectors this is called a linear combination. So, what we did here was took a linear combination of vectors r 1 r 2 up to r n. So, this c 1 r 1 plus c 2 r 2 plus up to c n r n is called a, this is called a linear combination of vectors, vectors r 1 up to r n. So, we took a linear combination and we said that if this linear combination yields and again I was a little sloppy there should be a 0 vector because linear combination of vectors gives you another vector because all we did was we multiply it by a scalar and we added it. So, we should get another vector. So, if this gives you a 0 vector, then if these vectors are linearly independent then this can only be satisfied if each of the c 1 up to c n equal to 0.

So, what that means is that the only way you can have this equal to 0, if all these are equal to 0. Now suppose vectors were r 1 r 2 up to r n were not linearly independent. So, if they were not linearly independent, or in other words they are linearly dependent then then; obviously, then the c 1 r 1 plus c 2 r 2 plus up to c n r n equal to 0 for some set such that c 1 c 2 up to c n such that not all of them are equal to 0.

So, for example, suppose c 1 not equal to 0. So, just suppose we can take any we can do with any of these scalars, but suppose c 1 was not equal to 0 then what you could do is you could write you could write r 1 as minus c 2 r 2 minus c 2 by c 1 r 2 minus c 3 by c 1 r 3 and so on up to minus c n by c 1 r n. You could write it as this we already said that c 1 is not equal to 0. So, c 2 by c 1 is the real number c 3 by c 1 is also real number and so on. So, all these are real numbers. So, what we did here is we expressed r 1 as a linear combination of r 2 r 3 up to r n.

So, what I want to tell you is that when vectors are linearly dependent, when they are not linearly independent then you can express one of them as a linear combination of the others. So, what we did what we what this rather obscure looking condition for linear independence implies is that you cannot write any vector as a linear combination of the others.

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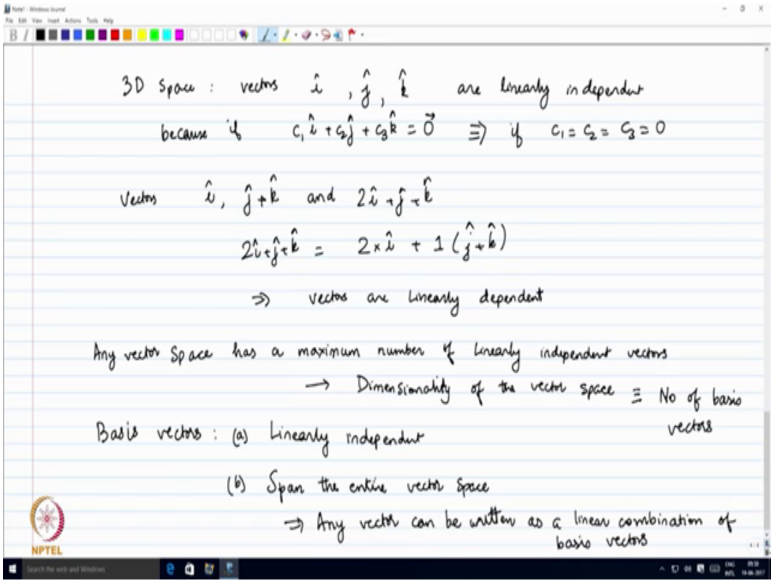

So, if you cannot write any vector as a linear combination of the others then the vectors are said to be linearly independent. So, for example, if you take the usual let us say in a 3D space. So, vectors i is also a vector j and k are linearly independent because if c 1 i plus c 2 j plus c 3 k equal to 0.

this implies this can only be true if c 1 equal to c 2 equal to c 3 equal to 0. So, if any of these are non 0 you will you cannot these cannot add up to 0. So, therefore, i j k are linearly independent vectors. Now what would be an example of vectors that are linearly dependent? So, for example, we can take we can take 3D vector space again. So, let us take let us take vectors i j let me take a vector j plus k, and let us say 2 y plus j plus k. So, I took these 3 vectors. So, I have one vector which is just i the other vectors j plus k and the third vector is 2 i plus j plus k.

Now, clearly I can write 2 i plus j plus k as 2 into i plus 1 into j plus k. So, I wrote this as a linear combination, I wrote this I wrote the third vector as a linear combination of the first 2 vectors. So, I took I multiplied the first vector by a by a scalar 2 and the second vector by a scalar one and I added them up. So, I took a linear combination of these 2 vectors, and I got the third vector. So, clearly these are linearly. So, implies vectors are linearly dependent.

So, the idea of linear independence and linear dependence is extremely important for in vectors and the if you take, if you take any vector space any vector space there are some they there is a maximum number of vectors that can be linearly independent, any vector space has a maximum number of linearly independent vectors.

So it has a maximum number of linearly independent vectors, and this is this is called the dimensionality, the t of the vector space. So, what that means, is that if you have a 2 dimensional vector space you cannot have 3 vectors that are linearly independent. So, in a 2 dimensional vector space you cannot have 3 linearly independent vectors. Similarly in a 3 dimensional vector space you cannot have 4 linearly independent vectors 4 or 5 or 6 or any number greater than 3. So, the maximum number of linearly independent vectors is equal to the dimensionality of the vector space and this is fairly obvious to see. So, you can just take any 3 vectors in 2D space and you can easily show that one can be written as a linear combination of the other 2.

Similarly, you can take any 4 vectors in the 3D space and show that one can be expressed as a linear combination of the other 3, but the point is that the idea of linear independence is related to the dimensionality of the vector space, now another way to say what the dimensionality of the vector space is to introduce the idea of basis vectors. So, your basis vectors, so basis vectors are set of vectors which are a linearly independent and b and the entire vector space. What does it mean by span the entire vector space; that means, any vector can be written as a linear combination of basis vectors.

So, basically if you know the basis vectors, then you can take a linear combination and you can construct any vector in the vector space. So, that is what you mean to span the entire vector space. So, if these 2 conditions are satisfied then the vectors are said to form a basis and these are called as basis vectors.

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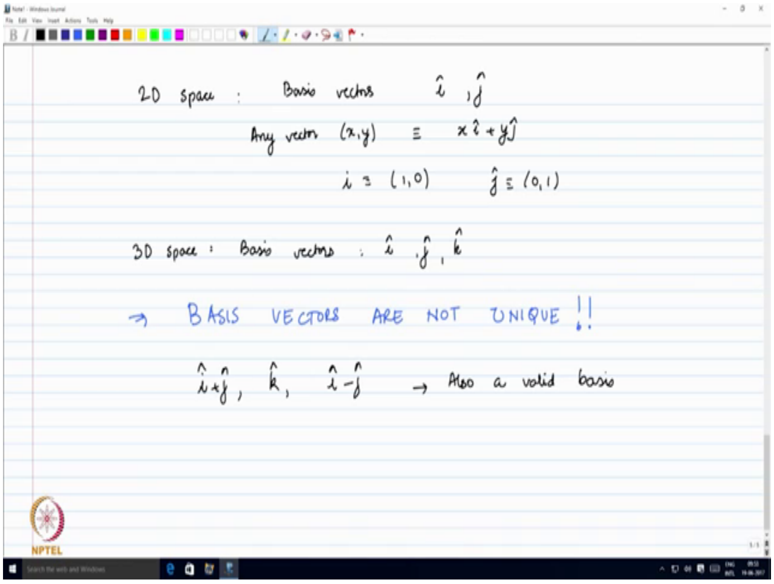

And now you will see that the dimensionality is equal to the number of basis vectors. So, the number of basis vectors is equal to the dimensionality of the space.

So, for example, if you take if you take a if you take a 2D space, you can choose basis vectors as i and j. So, any vector x comma y can be written as x i plus y j, I show did not mention this, but I can write I can write i as 1 0 and j as 0 1. I can write it in the same notation that we have been following I would be written as 1 0 and j would be written as 0 1. So, you can write any vector x y as a linear combination of i and j x times i plus y times j. So, these form a basis they are clearly they are linearly independent and you cannot have more than 2 linearly independent vectors in 2D space. So, they form a basis and you can write when they span the entire vector space.

Now, similarly in 3D space basis vectors are i j k this is this is one possible choice of basis vectors. Now importantly this is extremely important to note and I am emphasizing this here. So, basis vectors are not unique. So, this is a very important idea. In fact, in fact if we take 2D space, if you take any 2 linearly independent vectors they can form a basis. Any 2 linearly independent vectors in 2D space which span the entire space will form a will form a basis and in order to span the vector space they should be linearly independent and one of them should not be 0, and that is it you are done you can take any 2 linearly independent vectors and you can show that they span the entire vector space.

Similarly, any 3 linearly independent vectors in 3D will span the vector space and so they can be used as a basis. So, for example, in 3D, I can consider I can consider instead of instead of i j k as a basis I can take i plus j k i minus j, I can take these 3 as a basis. So, this is also a valid basis and you can check that these are linearly independent. And because the dimensionality of the space is 3 in 3D space these will span the entire space.

So, the idea of basis vectors and linear independence is actually extremely useful and what we will see in the next lecture is how this allows us to generalize 2 vectors of arbitrary dimensions.