Mathematics for Chemistry
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Module - 02
Lecture - 01
Vectors and scalars, Vector space, Vector Products

Welcome to module 2 of this course. So, in this module, I will be talking about vectors, vector spaces and vector functions and I will, there will be 4 lectures and one practice problem session. In the first lecture, I will talk about vectors and scalars vector space, vector products. In the second lecture I will talk about linear dependence, basis and dimensionality. In the third lecture, I will talk about vector functions, scalar and vector fields and vector differentiation and in the 4th lecture I will talk about gradient, divergence and curl which are 3 different ways of taking vector derivatives and then I will conclude in the fifth lecture with practice problems. So, each of the lectures will be about half an hour.

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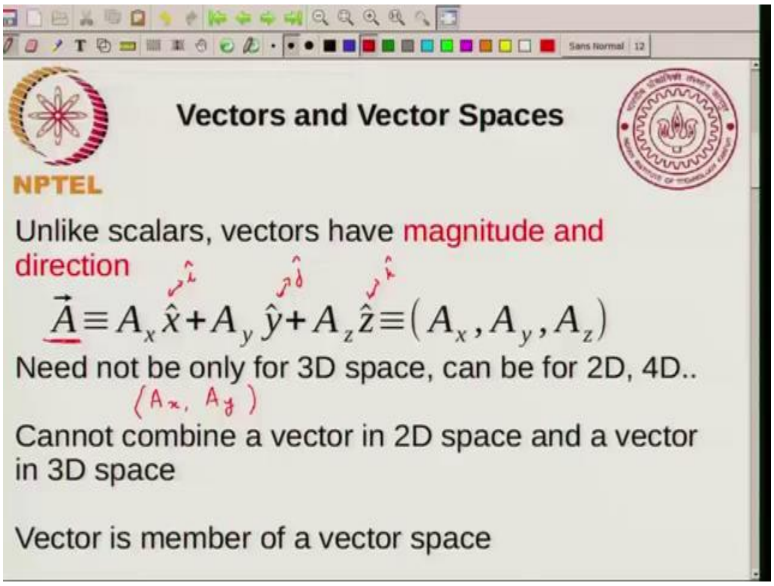

So, let us get started. So, in the first lecture I want to talk about vectors, vector space and vector products. So, all of you are familiar with the idea of vectors. So, what you know is that vectors have both a magnitude and a direction, unlike scalars which have only a magnitude. So, scalars have only a magnitude whereas, vectors have magnitude and a direction and so a typical vector you might write in this form, you might write a vector A as A x into x plus A y into y hat plus A z into z hat where, x hat, y hat and z hat alternatively you might write these as i hat, j hat and k hat. So, you are also used to this notation. So, you can write a vector in this form. So, A x, A y and A z are the components and sometimes instead of using a notation like this, you can just use a notation where you show a bracket A x, A y, A z where, you just show the components.

So, this is an example of a vector in a 3 dimensional space, but actually you can also have a vector in a 2 dimensional space. So, for example, suppose I just have A x, A y this is the vector in a 2 dimensional space. You could have a vector in a 4 dimensional space; you could have x, y, z, w you know you could have 4 dimensional vector space and there is nothing that stops you from defining vectors in 4, 5, 6 any dimensions, but what you will notice is that you have this idea of combining vectors. You can take 2 vectors and add them up, but if you take a vector in a 2 D space and a vector in a 3 dimensional space then; obviously, you cannot add them up. So, you cannot combine 2 vectors in different spaces in 1 and 2 D space and 1 and 3 D space or any 2 different spaces.

So, already with this idea we want to generalize and formally define a vector. So, formally if you want to define a vector you define a vector as a member of a vector space and what is the vector space? Will be the next question and that is what we will address next.

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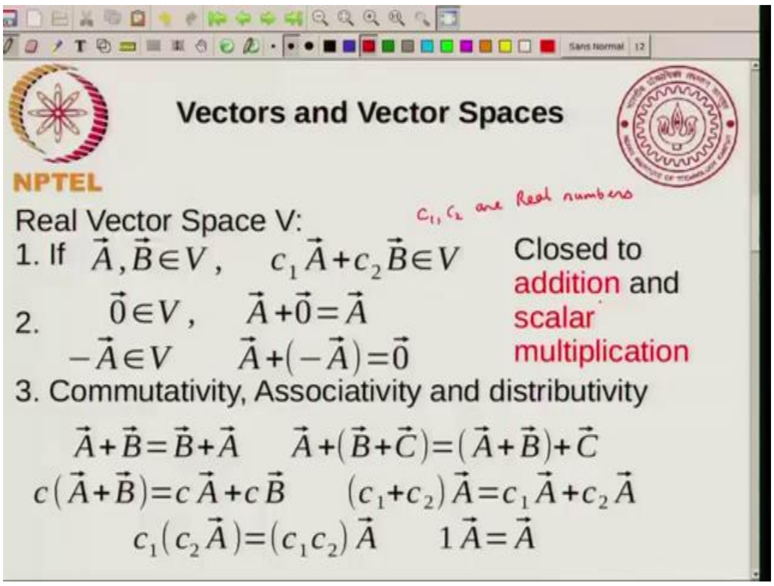

So, we need certain axioms that define a vector space. And we will look at these axioms next. So, real vector spaces V. So, these are the axioms of a vector space. So, what is a real vector space? You should keep in mind that a space is you can think of as a collection of objects. So, a real vector space is a collection of objects. So, it is a collection of objects called vectors. So, it is a collection of vectors and what are the properties of vectors? So, the properties are that if you have 2 vectors A and B which are in this vector space V then, you take a linear combination of them. You multiply by a scalar c 1 multiply A by a scalar c 1 and multiply B by a scalar c 2 and you will get another vector and c 1 and c 2 can be any real numbers. So, c 1 and c 2 are any real numbers.

So, the idea is that you can multiply this vector by any real number and add it to another vector multiplied by any other real number and you will still get a vector in the vector space. So, what it means? In short what you say the vector space is close to addition and scalar multiplication; that means, you add any 2 vectors, you will get another vector. You multiply a vector by a scalar, you will get another vector. Notice I am only talking about scalar multiplication; I am not talking about multiplication of vectors. So, the vector space is close to addition and scalar multiplication, that is the first axiom and the second axiom is that there exists a vector called 0 vector which is a member of the vector space V such that you can add it to any vector to get the same vector. So, A plus 0 gives you A and similarly there is a vector called minus A vector which is the inverse of A, such that if you take A and add minus A to it you get 0.

So, corresponding to every vector there is another vector of exactly the same magnitude, but opposite sign such that if you add these 2 vectors you get 0. So, these seem very obvious at least for the vector spaces we are used to dealing with, but. In fact, these are the very axioms on which the definition of vector space is based. The third axiom has to deal with Commutativity, Associativity and distributivity. I have combined bunch of axioms here. So, vector space addition is commutative. So, if you take A plus B it should be equal to B plus A. Similarly it is distributive if you take A plus B plus C, I can write that as A plus B plus C; again these are fairly obvious. Similarly scalar multiplication is also distributive.

So, suppose I take c into A plus B I can write as c A plus c B, alternatively if I take c 1 plus c 2 and multiply by A, I can write as c 1 A plus c 2 A. Similarly if I take c 1 into c 2

A, I can write as c 1, c 2 into A, again these are very obvious relations, but these are in fact, the formal conditions for a vector space. Similarly there is a scalar 1, if you just multiply 1 by A; you get A. So, why I want to go through this is that you know these kind of things are very obvious when you are dealing with vectors in 3 dimensional space, but in a lot of different areas, you will see vectors that are not necessarily vectors in 3 dimensional space and just to give you some examples.

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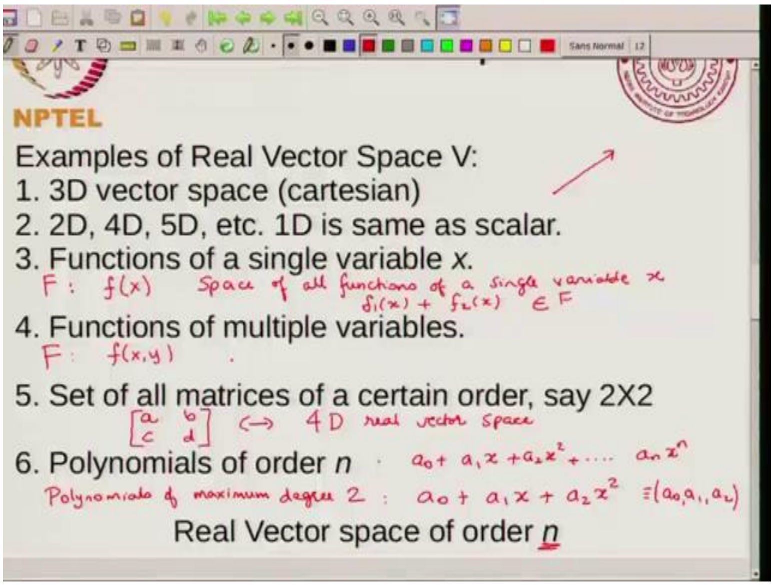

So, the examples of real vector space; so you know, the 3 D vector space, then or the Cartesian coordinates. So, you represented by a vector and you say that it has 3 components say in the X, Y, Z direction. You can have a vector in 2 dimensions as I said; you can have in 4 dimensions, 5 dimensions etcetera. Can you have a vector in 1 dimension? The answer is if you have a vector in 1 dimension is the same as a scalar because there is only 1 dimension. So, it only has a magnitude.

Now, you can also have a vector space consisting of all functions of a single variable. So, suppose you take some function of x and you take the space of all functions. So, F is the space of all functions; so f of x. So, is the space of all functions of a single variable? So, you imagine that you take any function of a single variable x. So, you imagine that you take any function of a single variable that is a member of this vector, that is a member of this space F and it is easy to show that F is in fact, a vector space because if you take one function f 1 of x and you add another function f 2 of x, you will clearly get another function. So, this is also contained in F.

So, you add 2 functions of a single variable; you do not get a function of 2 variables. You will still get a function only of a single variable similarly you do it, you multiply by a scalar you will get a function of a single variable. Similarly the 0 function is also a member of this vector space. So, you can define a function that is 0, which is also a function of x and. So, you can add it to any function and you will get back the function. Similarly you can also talk about inverse you can talk about and then; obviously, the Commutativity, distributivity properties are trivially satisfied.

So, the space of the set of all functions of a single variable that forms a vector space, similarly you can have functions of multiple variables, you can have space containing these functions of the form f of x y or f of x, y, z and that would also be a vector space. So, remember the vector space consists of all possible functions. So, it is a space containing all possible functions, just as you know you think of 3 D Cartesian space or a 3 dimensional space as the space of all possible vectors. So, you can have any vector and then the set of all possible vectors is what you call the space.

Similarly, you could take set of all matrices of a certain order. So, if I take any say 2 by 2 matrix. So, 2 by 2 matrix will would look like a, b, c, d; if I take the set of all possible. So, where a, b, c, d can be any real number if I take the set of all possible matrices then; obviously, if I add 2 matrices I will get another matrix, if I multiplied by a scalar I will get another 2 by 2 matrix. So, it is close to addition and scalar multiplication, you can define your 0 and so that is also a vector space.

Now, we can get to other things, you can say what about polynomials of order n. So, the polynomial of order n will look like a 0 plus a 1 x plus a 2 x square plus up to a n x raise to n and if you take the space of all possible polynomials of order n. Now if you take 2 polynomials of order n and add them up you will get another polynomial of order n. If you take 0 that is also you can also think of it as a polynomial of order n where all these coefficients are 0; a 1, a 2, etcetera. So, that is also member of the vector space. So, the set of the space of all polynomials of order n that is also a real vector space.

Now, you would intuitively realize that in order to, if you look at the space of polynomials right and let us just look for convenience, polynomials of order 2 of maximum degree 2 and the reason I am saying maximum degree is that, if I could also have. So, this is a general polynomial of degree 2 and the maximum degree I am saying is a maximum degree because if a 2 is 0, then it becomes a polynomial of degree 1; so polynomials of maximum degree 2.

Now, what you see is that you if I want to specify the polynomial, I just need to specify a 0, a 1 and a 2. So, I can write this as a 0, a 1 a 2 and. So, what you immediately realize is this is just like a 3 dimensional space because there are just 3 things you have to specify, 3 real numbers that you need to specify in order to specify any polynomial of maximum degree 2. So, actually it is equivalent, it is completely equivalent to a 2 dimensional vector space. There is no formally, there is no difference between these and. So, you can say that similarly this set of 2 by 2 matrices is equivalent to a 4 D; this is exactly equivalent to a 4 dimensional real vector space.

So, essentially if you say that when you say a real vector space of order of some order there is only one kind I mean all the real vector spaces of order n you can just call them n dimensional real vector space and. So, what I have say is that you have 3 D space, you have 4 D space, 5 D space, 6 D space, etcetera and what we will see later on is that, the dimensionality of the space of functions is actually infinite and we will give a formal definition of that. Now notice that when you see the axioms of a vector space, they only talk about addition of vectors and they talk about multiplication of vector by a scalar. So, they do not actually talk about multiplying 2 vectors and the reason for that is that there are many ways to multiplied 2 different vectors. So, there is not a unique way to define multiplication of vectors.

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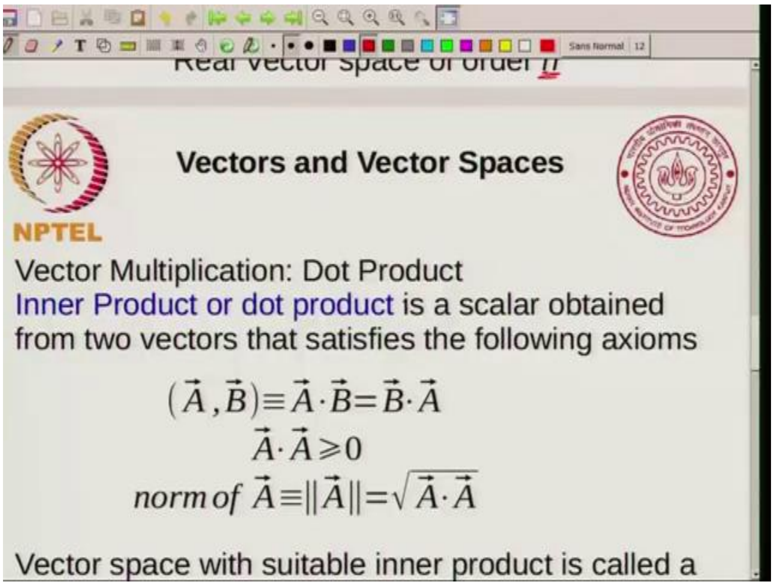

Now, there are some common things that you have seen already when you deal with vectors. So, there are certain kinds of products that you have seen; the dot product.

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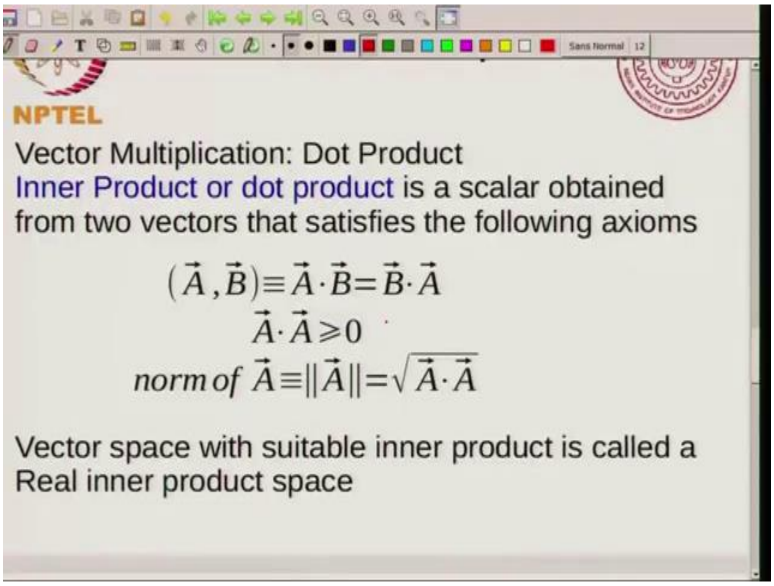

Now the dot product is also formally referred to as the inner product. So, the inner product is more general word for dot product. So, what is it? It is a scalar. So, inner product is a scalar that you obtain from 2 vectors and that should satisfy certain axioms. So, what are the axioms of an inner product? So, the inner product of A and B of 2 vectors A and B, so this is the inner product this is the notation. So, there are 2 ways to show it, you can show it either as A comma B or you can show it as A dot B. So, these are equivalent ways of saying is and. So, the inner product should satisfy that A dot B should be equal to B dot A.

So, what you do is you define a scalar. So, based on these 2 vectors you define a scalar and that scalar should satisfy A dot B equal to B dot A and it should satisfy A dot A should be greater than or equal to 0, any such definition is a valid inner product. So, any such definition of a dot product is a valid inner product and formally we define the norm of a vector as it is denoted by these double lines and that is just square root of A dot A. So, a vector space with a suitable inner product is referred to as a real inner product space and what I want to emphasize is that you can have vector spaces where inner product is not defined. There is no definition of a dot product or you can have vector spaces where dot product is easily defined, but formally real inner product space constitutes a vector space with a suitable definition of the dot product.

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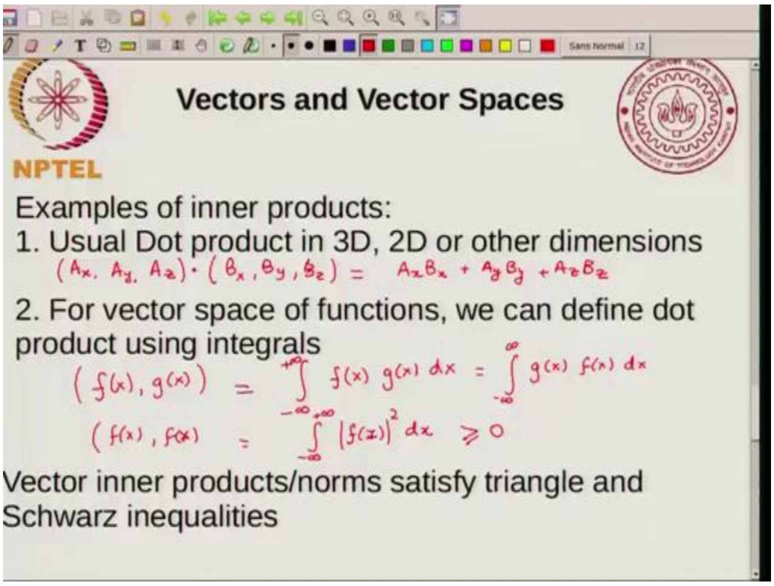

So, examples of inner products; so the usual dot product in 2 D or 3 D or other in 3 D vector space. So, suppose you have one vector A x, A y, A z and you have another vector B x, B y, B z; then their dot product is a scalar that is given by A x, B x plus A y, B y plus A z, B z and you can see that I can extend this definition to 2 dimensions or other dimensions to. I can use a similar definition for other dimensional vector space. So, this is one example of a dot product or an inner product.

Now, what about the vector space of functions? So, we talked about these functions f of x. So, suppose I have 2 functions, f of x and g of x; how do I define their dot product? So, you can define dot product, one definition is to say that the dot product of f and g it should be a scalar. So, dot product should be a scalar and you notice that it should be commutative. So, f dot g should be equal to g dot f and it should satisfy the norm condition. So, one way to define it is to say that f of x, g of x, d x over whatever the range of allowed values of x is. So, x goes from usually from minus infinity to plus infinity then I can define it this way. So, notice that this is equal to integral g of x, f of x, d x and also we notice that f of x comma f of x, this is equal to integral minus infinity to plus infinity. Now what you have is f of x square d x which is greater than or equal to 0. So, since the square of a function can has to be greater than or equal to 0, the integral of square of the function has to be greater than or equal to 0.

In fact, it is 0 only when f of x is 0. So, this is a valid definition of an inner product for a space of functions.

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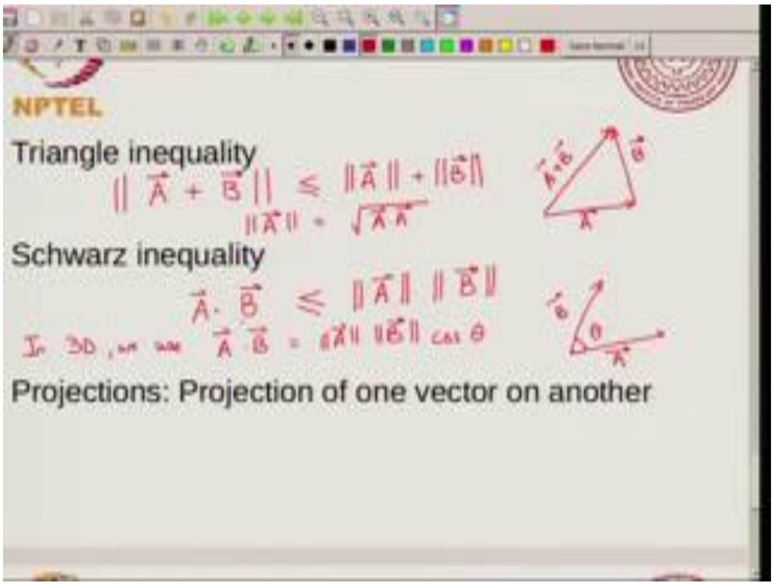

Now, the inner product defined this way, it satisfies the triangle and Schwarz inequalities. So, what is the triangle inequality? So, triangle inequality says that if you take 2 vectors A and B and you take the norm of A plus B. So, that should be less than equal to norm of A plus norm of B and what you think of is the following way. So, suppose you take A and you take B. So, this is A vector, B vector. Now you know that A plus B is nothing, but this vector, this is A plus B and so the norm the length of this plus the length of this should be greater than the length of this. So, that is called the triangle inequality and you know in 3 D space you are used to thinking of this as saying that you know sum of 2 sides should be greater than the third side, greater than or equal to the third side.

But this is a general relation for any. So, the norm of A just to remind you, this is square root of A dot A. So, it is defined in terms of the dot product and this is actually a property of a dot product. So, any dot product that satisfies the axioms of dot product will satisfy the triangle inequality. There is another inequality called the Schwarz inequality and that we can write in the following way. So, you can write A dot B, the norm of this of A or the I should not say the norm. So, what I should? I should just say A dot B, which is already a scalar. So, A dot B is a scalar and that is less than or equal to norm of A, norm of A is also a scalar multiplied by norm of B.

So, this is the Schwarz inequality and again you know in 3 D, we use A dot B is equal to norm A into norm B into cosine of theta where, theta is the angle between the vectors. So, you have A and B, if this is this angle theta then you are used to thinking of this dot product in this way and you know that or I should rather show it slightly differently. So, I will show it here, what I will do is I will show A and I will show B and this is theta. So, the angle between them and cosine of an angle has to be less than or equal to 1. So, we say that A dot B should be less than or equal to norm A into norm B.

Now, this again is generally true for an arbitrary vector space with an arbitrary inner product. Now the definition of dot product allows you to define something called a projection; projection of one vector onto another.

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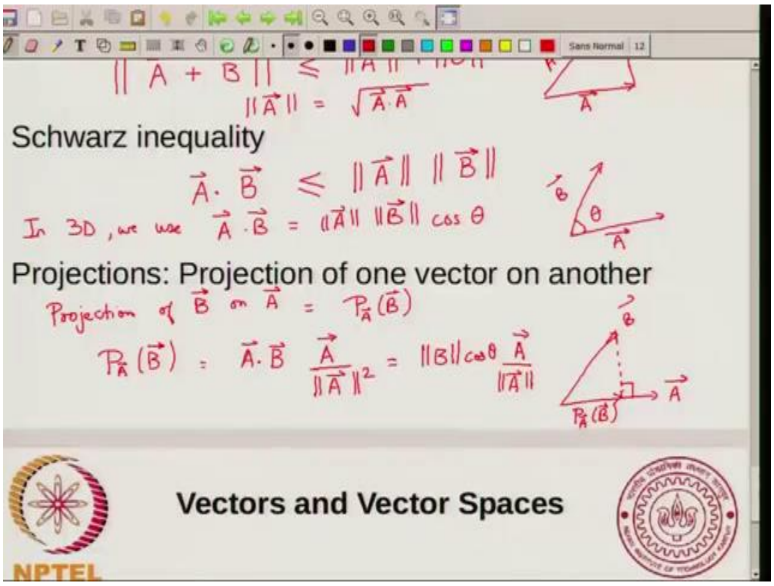

So, again suppose you have A vector and you have this is your B vector, you can define you can ask what is the projection of B onto A? So, if you in 3 dimension you know that if you drop a perpendicular from the end of vector B to vector A then this is called the projection. So, this vector is called projection onto A of B.

So, projection of B on A, this is written as P on A of B and you can again show from the dot product that P of can be written as A dot B multiplied by A vector divided by norm of A. So, it is not hard to show. So, you can think of this as just so it is B, the norm of B into cosine of theta. So, I can write this as, I am sorry there should be an A square. So, I can write this as just norm of B into cosine theta multiplied by a unit vector in the A direction. So, multiplied by unit vector in the A direction which is A vector divided by norm of A. So, this is the usual projection that you can define and again projection operators can be defined not just in 3 dimensional space, but in arbitrary vector spaces and again this is a very important tool in a quantum mechanics, the projection operator and vector spaces will play a very big role in quantum mechanics.

Now, there are other kinds of vector products that you can define and these are generally not as useful.

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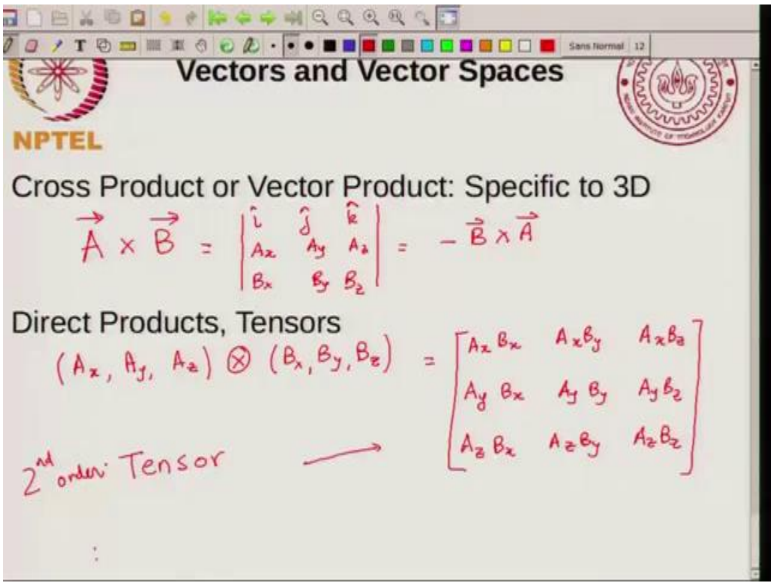

So, for example, the cross product; so A cross B, so this we usually write this as in terms of its components and. So, we write it as i, j, k and then you write A x, A y, A z, B x, B y, B z and this is equal to minus B cross A. So, this is not symmetric, now this is a vector. So, A cross B is a vector. So, it is also called a vector product this is very specific to 3 dimensions. So, you need to be able to write this in an anti symmetric form. So, this particular definition is specific to 3 dimensions and in general you know cross products are defined for odd dimensions, but usual cross products that we are used to seeing is defined for 3 dimensions. There are also other ways of taking products of vectors; one is called the direct product. So, just to remind, let us if I write a vector as A x, A y, A z and I write another vector as B x, B y, B z.

Now, what we are doing, when you are taking products of vectors is multiplying components. When you in the dot product, you multiply the x with x, y with y and z with z and you add them up. In the cross product what you do is you multiply x with z and y with z and subtract from z with y and that you call the x component. So, you generate vectors, but you can define products. So, I will just write the direct product and again there are many ways of defining direct products. So, one common way to define is to write this as A x, B x, A x, B y, A x, B z and then you can write it as A y, B x, A y, B y, A y, B z, A z, B x, A z, B y, A z, B z.

So, what you are doing is you are taking all possible products. You are taking x into x, x into y and so on and you are putting all of them in some sort of a matrix. This is referred to as a tensor. So, this is referred to as a second order tensor. So, second order tensor and. So, in this direct product, in this form of the direct product you get a second order tensor this way. There are other ways to define the direct product, but the why I wanted to show you the direct product is to show you where tensors come in and tensors are actually fairly useful objects in chemistry, I mean in quantum mechanics we often deal with the moment of inertia tensor. Similarly in studying spectroscopy, you will deal with the polarizability tensor and so on.

So, I will stop for here today. So, in the next lecture we will look at other properties of vectors, we will look at linear independence and basis and so on.