Advanced Mathematical Techniques in Chemical Engineering
Prof. S. De
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur

Lecture No. # 01
Introduction of Vector Space

Good morning everyone. So, welcome to the course of advanced mathematical methods in chemical engineering. We require several mathematical techniques, for solving of various chemical engineering problems.

Now, let us first try to understand, why do we require the mathematical methods? Why it is necessary for a chemical engineer? Now, any chemical process, it is if you would like to look into the production of any particular species, that will be involving lots of manpower material and there are several lots of fixed equipment.

So, to conduct one experiment successfully, you need to have huge investment. Now, if there is something wrong in the production, in the quality of the product, the whole batch will be waste. And the money involved in the manpower, money involved in the running the experiment, etcetera will be spoiled. So, there is a need of a modeling and simulation in actual chemical engineering process. So, let us try to understand, what is modeling and what is simulation and how it is related to mathematical methods in chemical engineering?

The modeling is basically required, when you would like to express - one as the particular process by writing the some characteristic of the process can be written in the form of some equations. The mathematical expression of the process is known as the modeling. So, once the model is properly done, then you must be simulating the process; so, you have to solve these equations. So, that you will be getting the output results in terms of (()) - let us say, conversion or in a temperature profile or some particular quality of the product so and so forth.

So, in order to solve these mathematical equations of modeled equation, you need to require the mathematical techniques. So, it is not possible to conduct the experiments number of times. So, that you can come to a conclusion, that this should be the appropriate operating conditions. So, that you will be getting the particular desired product in the output. So, in order to avoid that one has to conduct limited number of experiments and express the mathematical process in terms, express the chemical engineering process in terms of mathematical expression and try to solve them. And check whether these equations in the results of this simulation modeling and simulation by using the mathematical techniques whether, they are matching with the experimental data or not. If that is the case, then you can conduct a number of virtual experiments on the computer by simulation modeling and simulation and you can scale it up for a higher order of process. So that you can tell later on, that these are the typical operating conditions for which i will be getting the product, the quality of this the product of this quality.

So, therefore the mathematics will be used as a tool to solve the model equations of any chemical engineering processes. So, with this background, we start this chemical engineering course, the advanced mathematical techniques for chemical engineers and we will be starting with the vectors spaces and I will be mostly dealing with the analytical mathematics that will be most helpful for any chemical engineer in an actual plant operation.

Because there is another parallel category that is the numerical techniques, but that requires a different expertise and different setup in the computer etcetera. So, therefore, I will be mostly stressing on the analytical mathematics which will be very essential tool for the chemical engineers for solving the model equations for any chemical engineering process.

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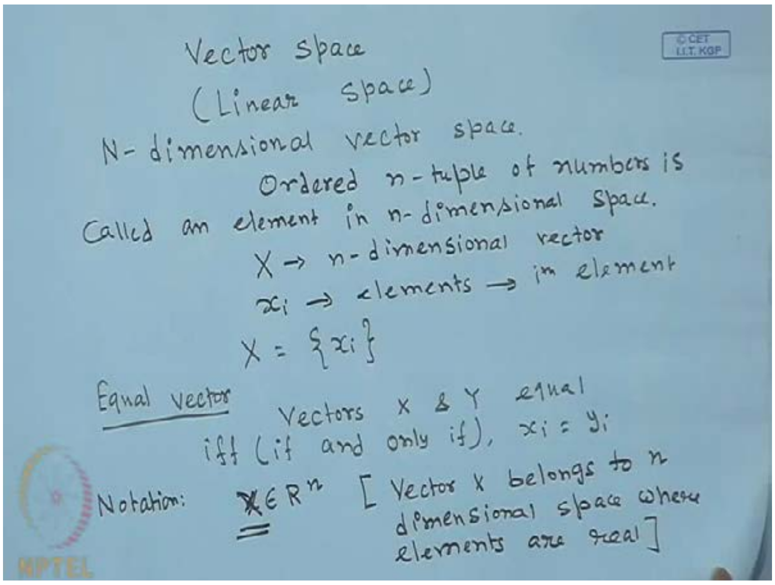

So, we will start with the vector spaces. This is also known as a linear space. Now, we talk about earlier, we know, we learned about the two dimensional vector space three dimensional vector space in this case we will be talking about N dimensional vector space.

So, what is the definition? The definition is ordered n-tuple of numbers is called an element in n dimensional space. The notation is that means, there are n numbers of elements in a vector. So, the notation is X is n-dimensional vector, if X is n-dimensional vector, then it will be having the elements x i small x i's so x i's are the elements and x i is the ith element. So, we write X is comprised of a set of element x i.

So, next we talk about the definition of what is an equal vector? We called the two vectors X and Y equal, if and only if all the corresponding elements of these two vectors will be identical. So, the notation i f f means, if and only if x i is equal to y i that means ith vector, ith element of the vector X and ith element of the vector Y. They are identical and equal.

Then, we have another notation, that is, X belongs to R is to the power n. This simply means, vector X belongs to n-dimensional real space, n-dimensional space - where elements are real.

So, vector X contains different elements which they which each every element is basically a real number. So, that is, why we called the real space and the vector X is called n-dimensional real space.

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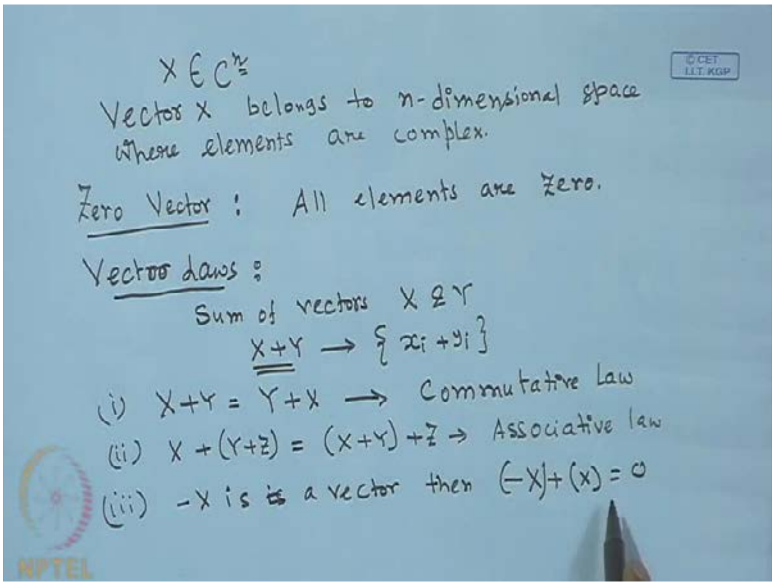

Next, we talk about, what is a complex space, if x belongs to C superscript n. This simply means, that vector X belongs to n-dimensional space. This n stands for dimension of the space. Dimension means, you will be having the contribution in n number of dimensions, which are mutually orthogonal to each other, vector X belongs to n dimensional space - where elements are complex.

Next, we call about a talk about a zero vector, what is a zero vector? The definition of a zero vector is that all elements of these vectors are identical to zero, then if all the elements are zero, then the constituted vector is called a zero vector.

Then, let us a rebrush refresh our ideas, our earlier definitions of vector laws, which most of us have studied during your ten plus two days and it may be earlier also that the sum of vectors X and Y that means X plus Y. This simply indicates that it is a new vector and the each every element of the new vector will be constituted by the corresponding elements of the two vectors and summing them up; that means, every element of this vector X new vector X plus Y is basically nothing but the summation of the corresponding ith vector of the individual vectors, then that will this that the set of these elements will constituted the vector X plus Y.

So, what are the laws, X plus Y is identical equal to Y plus X and this is known as commutative law.

Next, vector law is X plus Y plus Z. Suppose, there are three vectors X ,Y and Z and then these will be identical to X plus Y plus Z. This is known as associative law.

Next, vector law is if minus X is a vector, then minus X plus X will give rise to a 0 vector that means every element of minus X will be nothing but equal and opposite in sign to the corresponding elements of the X vector. So, when you add them up the whole addition will give rise to a vector where every element is zero; that is, why you will be landing up with a zero vector.

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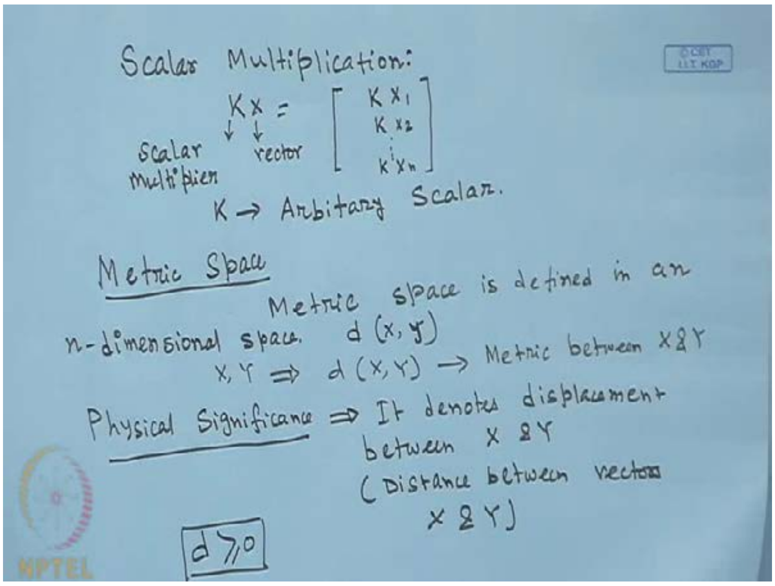

Then, we talk about the scalar multiplication, these simple operations and definitions will be quite useful, whenever we talk about, we go along the course of these particular slavers. K times X is nothing; X is the vector and K is the scalar multiplier, then every element of the X vector will be multiplied by the scalar K or let us say, X is the n-dimensional vector, then every element of the vector X will be multiplied by the scalar K and K is the arbitrary scalar.

Then, we talk about the three most important vector spaces in linear vector operations. First one is the metric space, so with these definitions, you will be able to solve lots of problem in chemical engineering problems and every case will be looking into some of the examples at the end of our lecture; so that it will be absolutely clear to the students, that how these mathematical techniques will be utilized for the chemical engineering applications for solving the actual chemical engineering processes.

So, what is a metric space? Metric is defined in an n-dimensional space, so we talk about a most generalized n-dimensional space. Suppose, there are n components in a chemical engineering process, then the space will be talking about is a n-dimensional space.

So, there is the most generalized one, if someone if in a system there are three components present, so it will be basically three dimensional space, if there are ten components present it is ten dimensional space. So, we talk about the most general, in generalized n dimensional space. So that the mathematical prob[lem]- problem the techniques that will be covering in this course, will be having a most generalized framework and any subset can be easily derivable out of these derivations.

So, what is the metric space? A metric space is defined in an n-dimensional space and the notation is d of X and Y, if X and Y are two vectors, then the metric between the two is denoted by d of X and Y. So, this is known as the metric between X and Y.

So, what is the physical significance of this metric? The physical significance of the metric is that it denotes displacement between vectors X and Y. In other words, it is nothing but the distance between vectors X and Y. So, that is the physical significance of the metric. Therefore, because of this definition one can understand that the displacement or distance cannot be a negative quantity, it will be a measurable positive quantity; therefore, d will be always greater than or equal to 0. If two vectors are identical the metric between the two vectors will be equal to 0, if not then there will be a definite metric existing between the two vectors X and Y.

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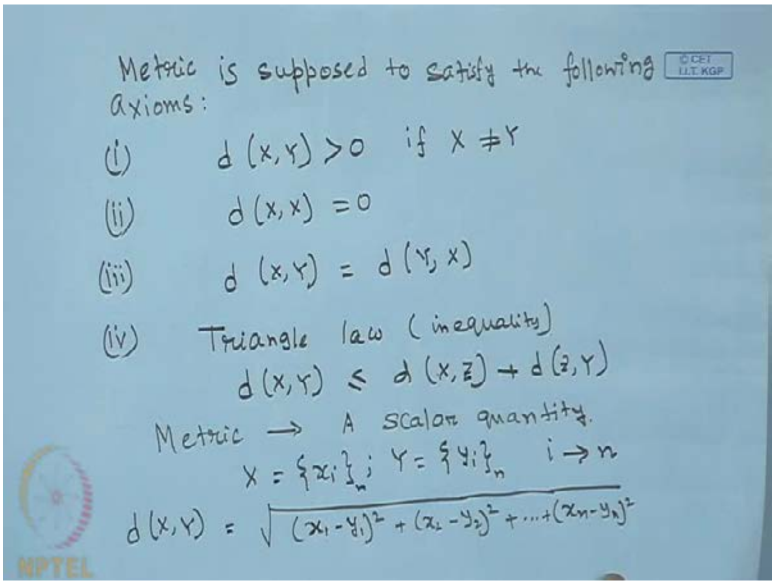

Now, let us look into some of the properties of the metric. So, the metric is supposed to satisfy the following axioms or set rules, what are these rules - the first axiom is that as i said earlier that metric is between two vectors X and Y will be always positive, always greater than 0, if X is not equal to Y; that means, if they are not identical vectors, then there will be a definite distance or displacement present between the two vectors X and Y.

Metric between X and X will be always equal to 0, this simply means that the distance between the X and X the same vector will be identically equal to 0; that means, the two vectors we are taking about in these cases are same.

Metric between X and Y will be nothing but metric between Y and X. So, this simply indicate if whatever the order between X and Y since metric basically a scalar quantity it giving a distance. Therefore, whether we talk about x and y or y and x. So, the distance between the two will always same.

The fourth will be basically the triangle law. The triangle law is that sum of two sides of a triangle is always greater than equal to compare to the other side. So, metric between X and Y will be less than equal to metric between X plus Z plus metric between X and Z and metric between Z and Y. This is also known as the triangle inequality law.

Therefore, we have understood that metric is nothing but a scalar quantity. So, it is a scalar characteristic defined between two vector quantities. Now, if there are two vectors, let us say X which will be constituted of x i and Y, which will be having the elements y i and i basically it goes up to n. Therefore, we are taking about an n dimensional space then what is the metric between X and Y, it is defined as under root x 1 minus y 1 square plus x 2 minus y 2 square and this goes on up to x n minus y n square.

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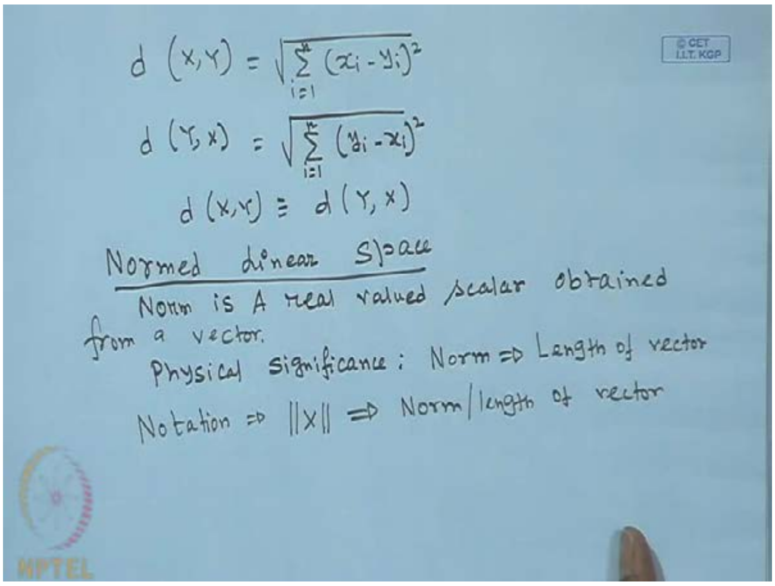

So, therefore, we can write it as in a short notation we can write the metric as d of X and between X and Y is nothing but under root summation x i minus y i whole square and where the index i runs from 1 to n, because the dimension is n and there are n number of elements presents in the system.

Similarly, we can talk about metric between Y and X is nothing, but under root summation i is equal to 1 to n y i minus x i square. So, if you look into these two expression, if the square whether it is a minus b whole square or b minus a whole square they are identical. Therefore, we prove the assumption the axiom metric between X and Y is identical with metric between Y and X.

So, that goes for the metric then we talk about normed linear space, next vector space is normed linear space. This is again, a real norm is nothing but a real valued scalar norm is real a valued scalar it is a real value scalar from obtained from a vector its physical significance is it gives norm represents the length of the vector and let us say, what is the notation? Notation is denoted by the two double bars.

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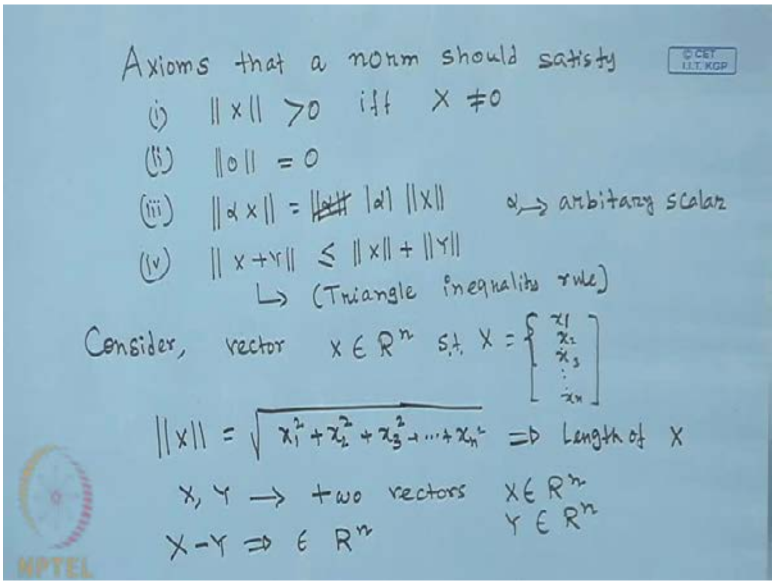

So, these means we are taking about norm or length of vector. Since, length does not have any direction, it is a scalar quantity. Again a norm must be satisfying some of set rules or axioms. Let us note them down, axioms that a norm should satisfy they are as follows: the first one, since it is a length norm is ever positive - if and only if X is not equal to 0.If X vector is not a zero vector, then norm of X vector is always greater than 0. Therefore, the next axiom follows that norm of a 0 vector is nothing but a zero vector. Third one is that norm of alpha X - where alpha is an arbitrary scalar. Then norm of alpha X is nothing but mod of alpha times norm of X.

Next assum[tion]- axiom is that norm of X plus Y is nothing but this is less than norm of X plus norm of Y again. This rule comes from triangle inequality rule. Next, we look into how the norm is define given a vector suppose, consider a vector X, such that X belongs to R superscript n that means X belong to a real number of space of dimension n. Therefore, X will constituting n numbers of real valued element x 1 x 2 up to x n.

So, therefore x will be compri[se]- you will be having n number of elements and every each one of them is a real valued number. Therefore, norm of X is defined as under root x 1 square plus x 2 square plus x 3 square plus up to x n square.

So, therefore, these this gives the length of vector X, hence it is a scalar quantity. Now, if we look into another vector, let us say X and Y are two vectors, each of it is they belong to the n-dimensional real space that means X belongs to n dimensional real space and Y it belongs to n-dimensional real space, then we defined a vector X minus Y.

So, therefore, X minus Y is a vector that belongs to n-dimensional real space as well that means, what is X minus Y? X minus Y is nothing but it will be a vector in n-dimensional space, where every element of this vector will be nothing but x 1 minus y 1 x 2 minus y 2 like that and up to X n minus Y n.

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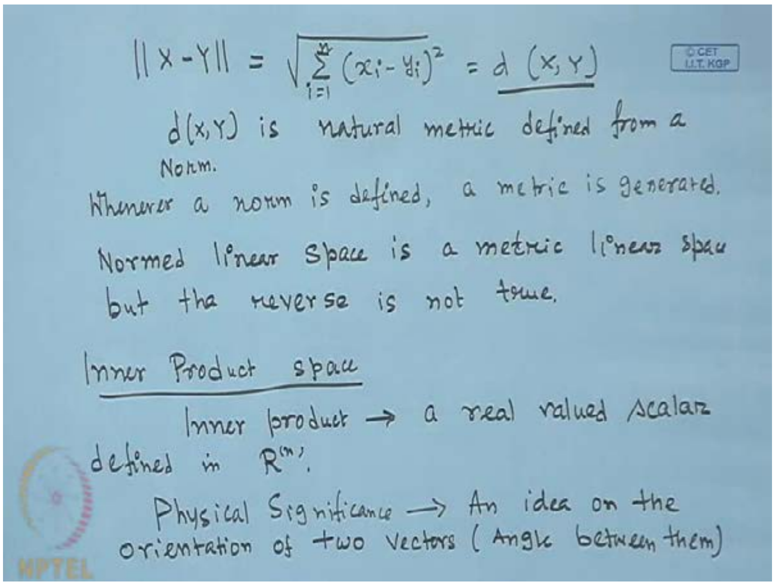

So, what will be the norm of the new vector X minus Y. The norm of new vector is nothing but under root summation and this summation goes from index i equal to 1 to n and this will be x i minus y i square.

Now, if you look into the definition of metric, what is this under root summation x i minus y i square. This is nothing but the metric between the two vector X and Y.

So, therefore, if we look into these very closely. So, d metric is called it is a natural metric, defined from a norm therefore, whenever a norm is defined a metric is generated

So, therefore, whenever we will be defining a norm a metric will be naturally derived automatically generated. So, therefore, we can come to a conclusion that normed linear space is nothing but a metric linear space but the reverse is not true.

That means whenever a norm is defined a metric is generated, but whenever a metric is generated; we cannot define a norm. So, it is not from metric to norm but it is the other way round it is from norm to metric. So, whenever we will be defined a norm a metric is automatically generated.

Next, linear vector space we talk about the inner product space. Let us look, into the definition of inner product - inner product is again a real valued scalar defined in n-dimensional real space and what is the physical significance of inner product?

The physical significance of the inner product is that physically it indicates the angle between the two vectors X and Y. So, it gives, an idea on the orientation of two vectors in more specific terms it gives the angle between them.

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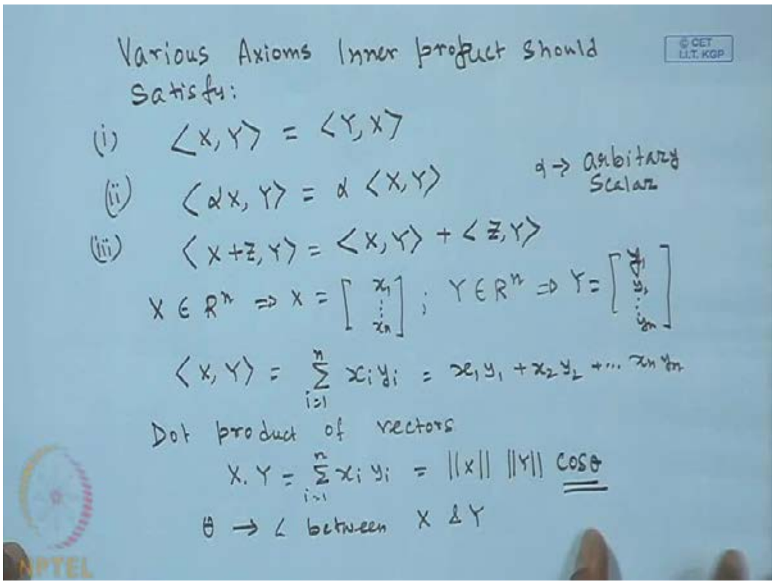

So, let us look into the various axioms that inner product should satisfy or axioms or properties the inner product should satisfy are as follows : the first one is that inner product between X and Y is identical between inner product that of inner product between Y and X that means the orientation of X and Y and orientation of Y and X they are same and equal identical.

Second one is if the inner product if the vector X is multiplied by a scalar alpha and then inner product between alpha X and Y is nothing but alpha multiplied by inner product between X and Y where alpha is a arbitrary scalar.

Next one is if there are three vectors belonging to the n dimensional real space X Y and Z then inner product between X plus Z and Y should be the inner product between X and Y plus inner product between Z and Y.

Now, let us look into how to compute inner product between two vectors X and Y. X belongs to n dimensional space constituted of the elements x 1 up to x n.Similarly, Y is another vector belongs to n dimensional real space, such that Y is constituted by the elements y 1 y 2 up to y n.Then inner product between X and Y is nothing but summation of the corresponding elements to multiply the corresponding elements of the two vectors X and Y and then and sum the sum them up for all the elements. So, it will be nothing but x 1 y 1 plus x 2 y 2 up to x n y n.

So, this is nothing but the dot product of two vectors X and Y. So, what is the dot product of X and Y. This will be nothing but summation x i y i therefore this will be nothing but norm of X multiplied by norm of Y multiplied by cosine theta - where theta is the angle between the vectors X and Y.So, therefore, if we know vectors X and Y, then their dot product or the inner product will be giving you the angle between them cosine theta - where cosine theta is nothing but the inner product between the two vectors divided by norm of X multiplied by norm of Y.

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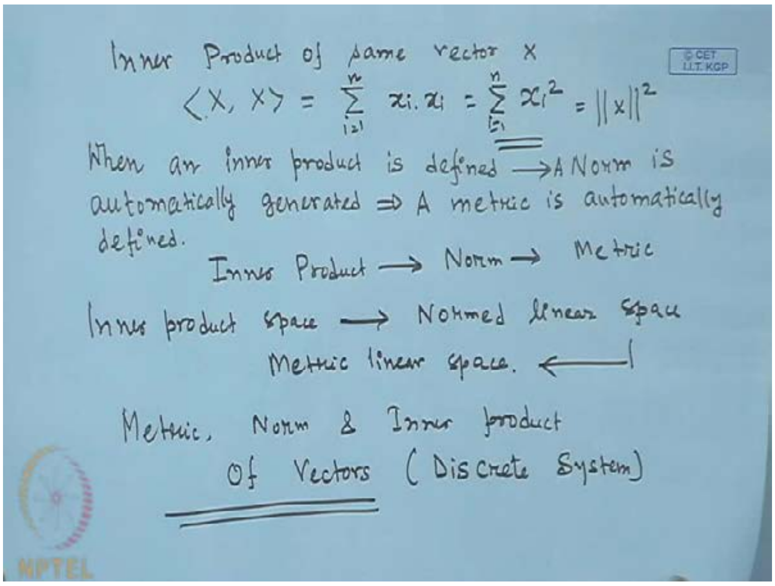

So, if you look into the inner product of the same vector. Let us say X, so inner product between the same vector is nothing but if you put the substitute, the definition of the inner product so this will be for summation over all the elements i is equal to 1 to n this will be X Y Y Y, if we are talking about two vectors X and Y; therefore this will be nothing but x i multiplied by x i so this will be summation of x i square i is equal to 1 to n and what is this definition this is nothing but norm of X square of that this is nothing but square of norm.So, therefore, if you look into this, so what is the interpretation? The interpretation is that when an inner product is defined, we will be getting a norm is automatically generated and we have seen earlier that when a norm is automatically generated, a metric is automatically generated defined. Therefore, whenever we will be talking about an inner product we will be getting a norm and then we will be getting a metric.

So, therefore, definition of inner product, simply indicates that a norm is defined and a metric of a vector is defined. So, therefore, we can talk about that inner product space it say more general space, then from that we will be getting a normed linear space, then we will be getting a metric linear space.

So, these three spaces are differ; so basically in inner product, norm and metric are the three scalar quantities. One will be getting out of the vectors and they will be quite important. As far as the mathematical treatment of various systems in chemical engineering processes are concerned, that we will see as we go along the course along and the various rest portion of this course.

Now, what we have done till now? We have looked into the norm, how to define metric norm and inner product of vectors. where each of So, vector is nothing but a discrete system that we have seen, that if a vector is given n-dimensional generalized vector either in real space or in complex space, then how will you generate the metric norm, how will you mathematically express the expression of metric norm and inner product?

Now, next we will see that the if the space if your system is not a discrete system, let us say it is a continuous system and what is a continuous system - represented a continuous system is represented by continuous functions.

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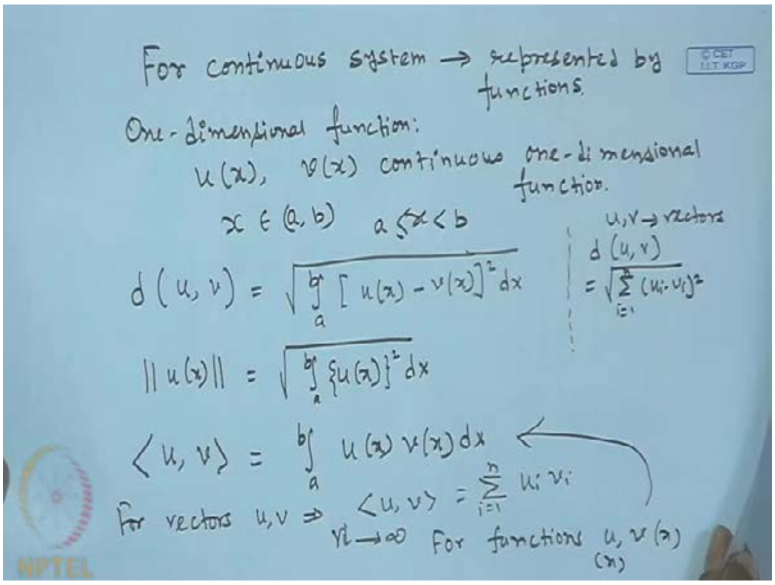

So, for continuous system it is represented by functions, again these functions can be one dimensional functions, two dimensional function, three dimensional function.

So, let us consider first a one dimensional function, what is the one dimensional function? One dimensional function is nothing but the function that it is an expression, which is a function of only one independent variable let say x.

So, u of x v of x they are basically continuous functions and their examples of continuous one dimensional function.

Now, let us say x belongs to a and b, this gives the domain or the limit of x that means x varies between a and b.

So, what is the metric of u and v? In this case, for the continuous function metric between u and v is defined as under root integral a to b u of x minus v of x square of that d x. If you remember, if you look into the corresponding definition of metric for discrete domain, for example, for the case of vectors then d of u and v is nothing but under root summation u i minus v i square, if u v u v are vectors.

Now, whenever these particular elements they are closed spaced, let us say these vectors their of particular elements are closed spaced, then they will be represented by the functions; so you will be getting the summation. In the case of function, this summation will be represented by this integral over the domain between a and b and you will be getting these expression.

So, similarly, norm of u is nothing but under root a to b u of x square of that d X, that is, the definition of norm of u. Similarly, you will be getting norm of v as under root a to b v of x square multi[plied]- times d X.

Then inner product between u and v is nothing but the integral of u of x v of x d X. So, for discrete for vectors u and v, the inner product between u and v is nothing but i is equal to 1 to n summation u i v i, when these i tends to infinity then the n tends to infinity, then this discrete domain will be simulated by the continuous domain. Therefore, for functions u and v, which are the continuous functions in x will be getting the inner product by this expression integral a to b u x v x d X. So, this is the definition of the three vector space, inner product, norm and the metric, if we have continuous one dimensional function.

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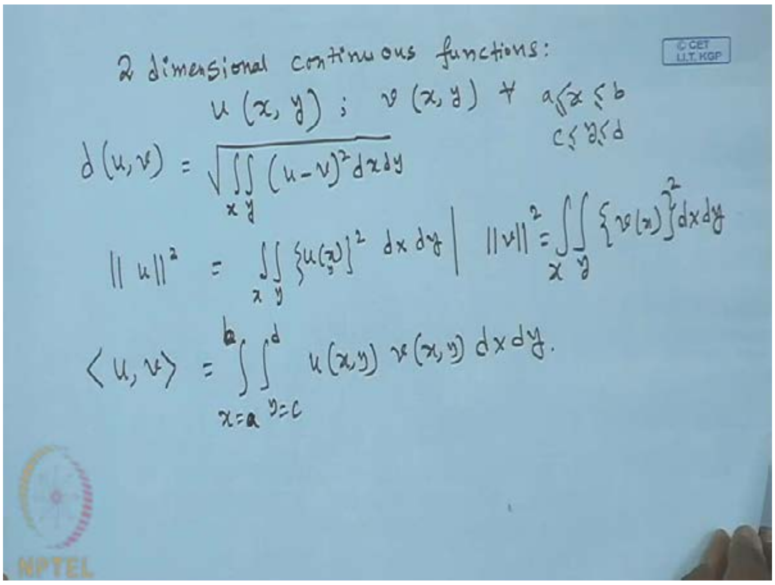

Now, let us talk about a for two dimensional continuous functions that means, if we have functions u as a function of x and y v as a function of x and y then metric between u and v is nothing but under root. Let us say, x lying between a and b y lying between c and d, then since it is a two dimensional space, two dimensional function. So, therefore, these integral will be represented by a the single integral replaced by a double integral u minus v whole square d x d y.

The norm of u will be nothing but integral over x integral over y u of x x and y square of that d X d y. Similarly, one can define norm of v, as integral over x integral over y v of x square of that d X d y. And the inner product between u and v will be nothing but double integral x from a to b y from c to d u of x y multiplied by v of x y d X d y for a three dimensional problem this function the functions u and v will functions of three independent dimensions x y and z so in that case the limits of x y and z will be defined and they will be prescribed.

So, one can get the metric between u and v as under root triple integral. This double integral will be replaced by the triple integral in that particular case and it will be triple integral over x over y over z u minus v whole square d X d y d z.

Similarly, norm of u will be defined as triple integral u of x y z square d X d y d z and inner product between u and v as triple integral u multiplied by v d X d y d z. So, we have seen that how norm the linear metric, the vector spaces like norm metric and inner product are defined in one dimensional continuous function, in case of discrete domain in vectors in continuous domain, one dimensional function, two dimensional function and three dimensional function.

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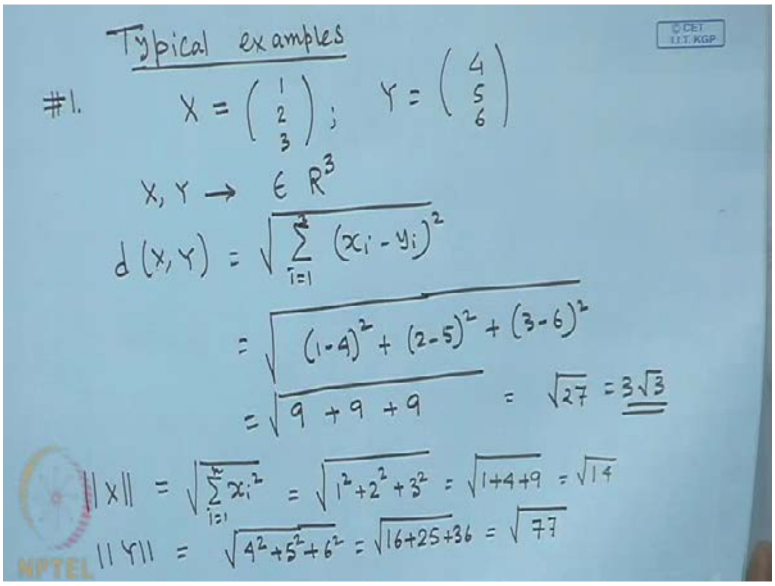

Next, we look into some of the typical examples then computation of these things will be absolutely clear. The first example will be let us consider a vector X as 1 2 3 and Y as 4 5 6. So, basically X and Y are they are vectors they each of they belong to three dimensional real spaces. So, we compute the metric between the vectors X and Y, we compute the norm of X and norm of Y and we like to compute the inner product between X and Y.

So, what is the metric between X and Y it will be simply summation under root summation between 1 2 3 i is equal to 1 2 3 because there are three elements, x i y i square of that we just replace the you know write down the definition

So, this will be under root 1 minus 4 square of that plus 2 minus 5 square of that plus 3 minus 6 square of that. So, what will be getting is minus 3 square; so it is 9 plus minus 3 square so it will be 9 plus minus 3 square; so it will be 9 so you will be getting root over 27 or 3 root 3 that is the metric between the vectors X and Y. So, it is the distance between the vectors two vectors X and Y.

Next, we define what is norm of X, if you look into the definition of norm, it is nothing but this is for general definition of a norm of n dimensional vector X, it is under root summation of x i square but the index i runs from 1 to n.

So, in our for this particular example, it is a three dimensional space. So, it will be under root of 1 square plus 2 square plus 3 square, it will be 1 plus 4 plus 9; so it will be root over 14 units

Similarly, we can go for norm of vector Y and this will be 4 square plus 5 square plus 6 square. So, this will be root over 16 plus 25 plus 36 and this will be 16 plus 25 is 41. So, it will be root over 77 units so that will be the norm of Y.

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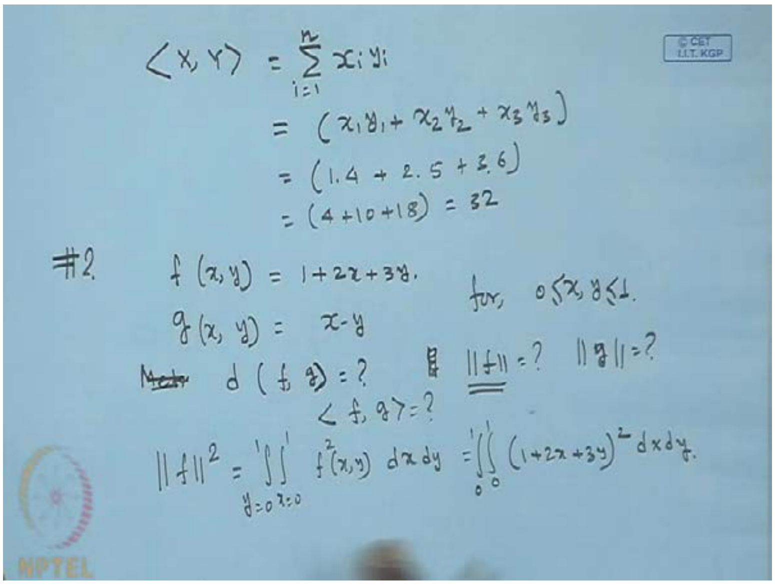

And similarly one can compute the inner product between X and Y. The inner product between X and Y, if we write the general formula it will be summation of x i y i, where the index i goes form 1 to n that means both X and Y are n dimensional vector.

Now, if we look into our example, so this will be x one x 1 y 1 plus x 2 y 2 plus x 3 y 3. So, it will be 1 into 4 plus 2 into 5 plus 3 into 6 it will be 4 plus 10 plus 18 so as you 14 plus 18 this is of 32 units.

That is how, whenever this simple example gives that if a vector is given finite dimensional vectors -three dimensional vector, four dimensional vector, then you will be these are the simple mathematical operations by which one can compute the norm inner product and the metric between the vectors.

Next, we take up an example of a continuous domain. So, the earlier example is for the discrete domain in case of vectors next we take up with the for the continuous domain. Let us say f of x y is 1 plus 2 x plus 2 y and g of x plus y is x minus y and in both the cases x and y, they are varying between 0 and 1. So, the limits of x and y from 0 and 1.

So, let us look into how will you get the metric between our idea, what is the metric between f and g, what is the norm of f, what is the norm of g and what is the inner product between f and g?

Let us first look into what is a norm since it is a two dimensional function then this norm is nothing but represented by a double integral. So, norm of f square of that is nothing but integral one integral over x from 0 to 1 another integral over y from 0 to 1 f x y square of that d x d y. So, this will be basically from 0 to 1 from 0 to 1 1 plus 2 x plus 3 y square d X d y.

So, basically you have to carry out this integral and find out the answer, so if we really carry out this integral, so let us see what we get.

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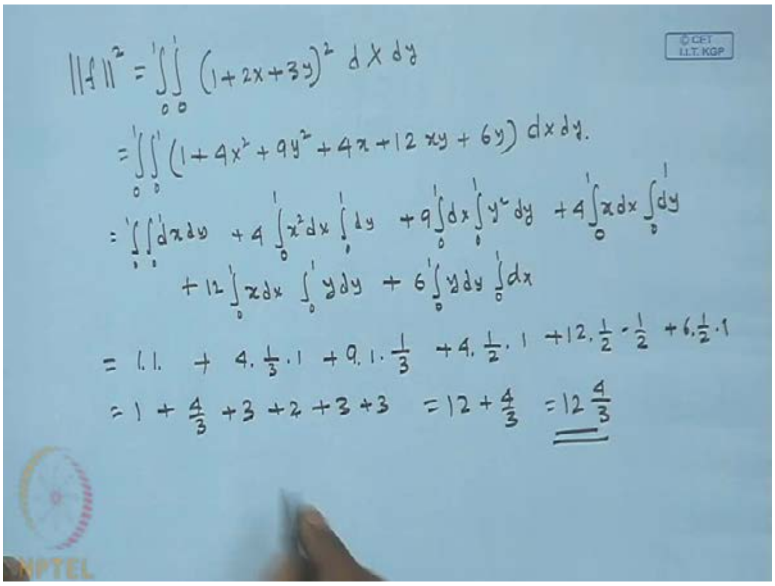

Norm of f square is that 0 to 1 integral 0 to 1 0 plus 2 x plus 3 y square of that d X d y just open up this square. So, it will be 1 a square plus b square plus c square plus 2 x y so it will 4 x plus 3 into 2 6 to 12 x y plus 6 y d X d y.

So, d x d y 0 to 1 0 to 1 plus 4 x square d X 0 to 1 d y 0 to 1 plus 9 0 to 1 d X y square d y 0 to 1 plus 4 x d X 0 to 1 0 to 1 plus 12 0 to 1 x d X 0 to 1 y d y plus 6 y d y 0 to 1 multiplied by d x 0 to 1.

So, the first integral will be 1 multiplied by 1 second integral will be 4 1 upon 3 multiplied by 1 9 into 1 into 1 upon 3 plus 4 into 1 upon 2 into 1 plus 12 into 1 upon 2 into 1 upon 2 plus 6 into 1 upon 2 multiplied by 1.

So, you will be getting 1 plus 4 by 3 plus 3 plus 2 plus 3 plus 3 three 3 3 6 6 2 8 8 3 11 11 1 12 12 plus 4 by 3 so you will be getting a 4 by 3. So, this the norm of the continuous function f likewise you have to carry out the other parts. and in the I will stop here in the next class will be solving this problem completely.

Thank you very much.