Advanced Mathematical Techniques in Chemical Engineering

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Lecture No. # 05
Vectors (Contd.)

Well, in this class, what we had discussed in the last class is that, we were looking into the Gram-Schmidt orthogonalization technique. This technique is in use rampantly for the orthogonalization and orthonormalization of independent set of vectors, which will later on simplify the calculation, calculation complexity of any other vectors, which will be expressed as a linear combination of all the independent set of vectors.

So, we will continue with the Gram-Schmidt orthogonalization technique for that, so what we have done in the last class, we considered a set of independent vectors h 1, h 2 up to h k in a k dimensional space and we would like to constitute a set of vectors e 1, e 2, e 3 up to e k, where each of these vectors in the target set; we call that e set is the target set. In this target set, all these vectors will be independent, as well as they are mutually orthogonal and orthonormal.

We have formulated the first element of the e set, the target set e 1; e 1 is nothing but h 1 divided by norm of h 1 ensuring that the e 1 will be having a norm unity and we have already proved that.

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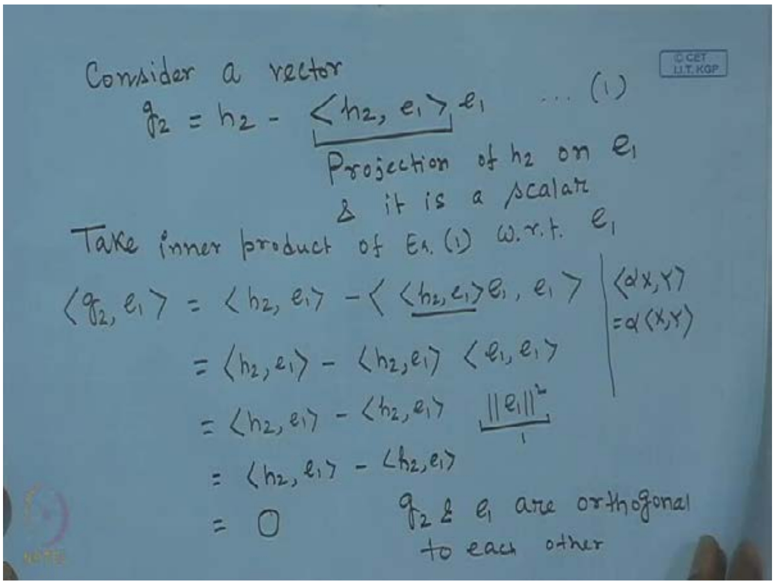

Now, in this class, we will be formulating the other elements of the target set e 2, e 3 onwards. So, in order to get the e 3 we have to consider a vector g 2, which is nothing but h 2 minus inner product of h 2 and e 1 multiplied by e 1. So, inner product is nothing but, since, it is nothing but a scalar multiplier, we can formulate this vector in this particular form.

Now, what we can do? We take inner product of this equation with respect to vector e 1. So, if we do that this becomes inner product of g 2 and e 1 is equal to inner product of h 2 and e 1 minus inner product of h 2, e 1, e 1 with e 1. So, this becomes inner product of h 2 and e 1. In this equation h 2 and inner product of h 2 and e 1 is nothing but a scalar and if we remember the property of the inner product that if it is inner product of alpha x and y, where alpha is a scalar multiplier, then this should be alpha times inner product of x and y.

We take this inner product, the scalar multiplier h 2 e 1 out of this and this becomes inner product of e 1 and e 1 and inner product of e 1 and e 1 is nothing but the norm of e 1. This is nothing but the norm of e 1 and we have already ensured that norm of e 1 is equal to 1. So, therefore, this value will be equivalent to 1. This will be inner product of h 2 and e 1 minus inner product of h 2 and e 1. These two scalars are identical and opposite in sign, so that will be equal to 0. This simply indicates that the inner product of vector g 2 and e 1 will be equal to 0. If you remember the last class, if that is the condition then we can come to a conclusion that g 2 and e 1 are orthogonal to each other; this simply indicates that g 2 and e 1 are orthogonal to each other.

So, we get the second vector of the target set e, but we cannot ensure at this point of time that g 2 and e 1 are orthogonal that is fine, but g 2 is not orthonormal, we have to make the norm of g 2 to be 1 to make it an orthogonal - orthonormal set.

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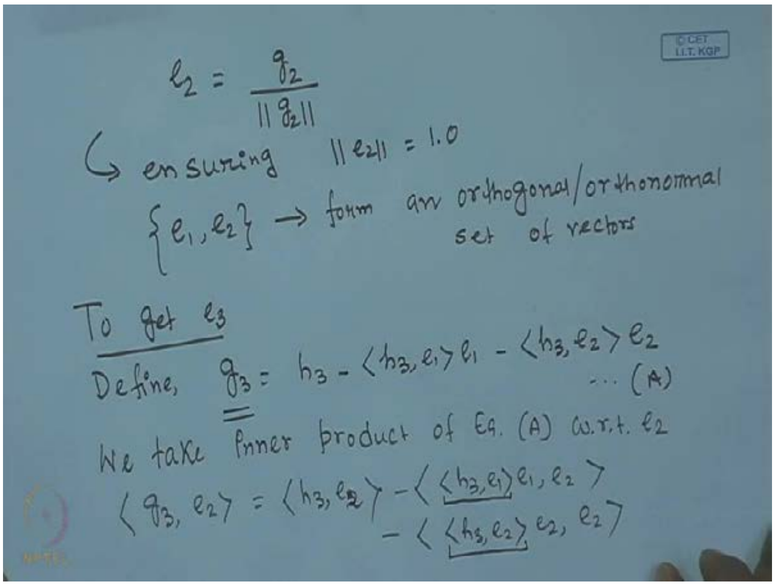

The next element of the target set e 2 is nothing but g 2 divided by norm of g 2. So, this ensures that the norm of e 2 is equal to 1. We are doing this to ensure norm of e 2 is equal to 1.So, now, e 1 and e 2 constitute an orthogonal and at the same time orthonormal set of vectors.

So, we have already obtained two elements of our target set; next one is to get e 3. We would like to obtain the next element of the target set, for that we define, g 3 as h 3 minus inner product of h 3 and e 1 e 1 minus inner product of h 3 and e 2 multiplied by e 2. We consider this vector g 3 is equal to h 3 minus a scalar multiplier with respect to e 1 minus another scalar multiplier with respect to e 2, but this multiplies nothing but the inner product of h 3 and e 1 and this multiplier is nothing but inner product of h 3 and e 2.

Now, we take the inner product of this equation (Refer Slide Time: 07:00). Now, we will be saying that g 3 will be orthogonal to e 2. In order to prove that we have to take the inner product of this whole equation, let say, this equation number A with respect to e 2. If that inner product turns out to be 0 then, we can come to a conclusion that g 3 is orthogonal to e 2. So, we take inner product of equation A with respect to e 2. So, this becomes inner product of g 3 and e 2 should be is equal to inner product of h 3 and e 2 minus inner product h 3, e 1 e 1 and e 2 minus inner product of h 3, e 2 e 2 and e 2.

Now, again, we will be utilizing the properties of the inner product that inner product of alpha x and y is equal to alpha and multiplied by the inner product of x and y, where alpha is a scalar multiplier. Again, inner product is always a scalar, this is a scalar multiplier and this is another scalar multiplier. So, they can be taken out of this bigger inner product sign (Refer Slide Time: 08:26).

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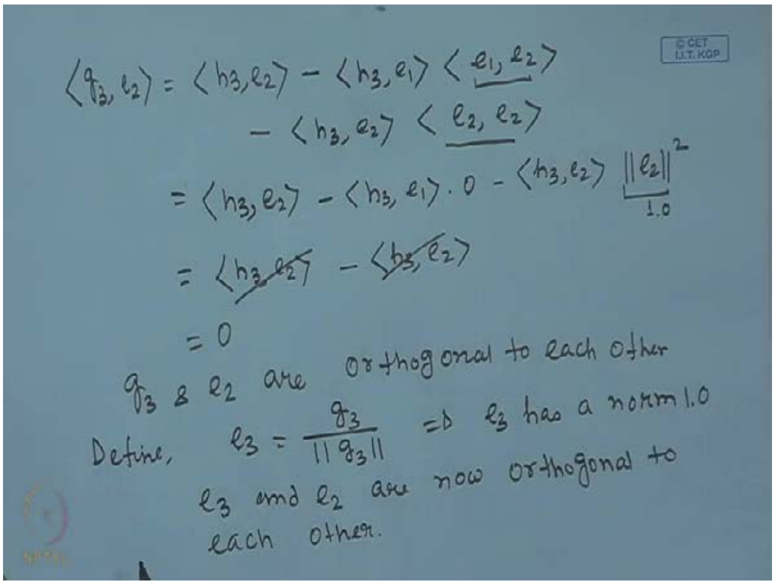

So, if we do that this becomes inner product between g 3 and e 2 should be equal to inner product between h 3 minus e 2 minus inner product of h 3 and e 1 is a scalar therefore, it will be out of the a larger inner product sign, so this will be inner product between h 3 and e 1 multiplied by inner product between e 1 and e 2 minus h 3 and inner product of h 3 and e 2 being a scalar will be taken out and this will be inner product of e 2 and e 2.

Let us see, what we get? This is inner product of h 3 and e 2 minus inner product of h 3 and e 1 and we have already said and proved that e 1 and e 2 are mutually orthogonal to each other, so therefore, inner product of e 1 and e 2 will be equal to 0, this will be equal to 0 minus inner product of h 3 and e 2, what is inner product of e 2 and e 2, it is nothing but the norm of e 2, we have already proved earlier that e 2 is defined such a way that the norm is 1, so this will be unity. So, what we get? We get inner product of h 3 and e 2 minus inner product of h 3 and e 2; these two being scalar and opposite in sign, they will be simply cancelled out and there will be equal to 0.

This proves that g 3 and e 2 are orthogonal to each other, but it does not a confirm that norm of g 3 is equal to 1; Still now, it is an orthogonal set but not an orthonormal set. So, we have to make g 3, we have to normalize g 3 to make its norm 1. So, for that we define e 3 such that e 3 is nothing but g 3 divided by norm of g 3. So, this ensures that e 3 has a norm 1.

So, therefore, g 3 e 3 is directly derived from g 3; e 3 and e 2 will be mutually orthogonal to each other; so, e 3 and e 2 are now orthogonal to each other. We have already proved that e 1 and e 2 are orthogonal, e 2 and e 3 are orthogonal; therefore, e 3 and e 1 have to be orthogonal.

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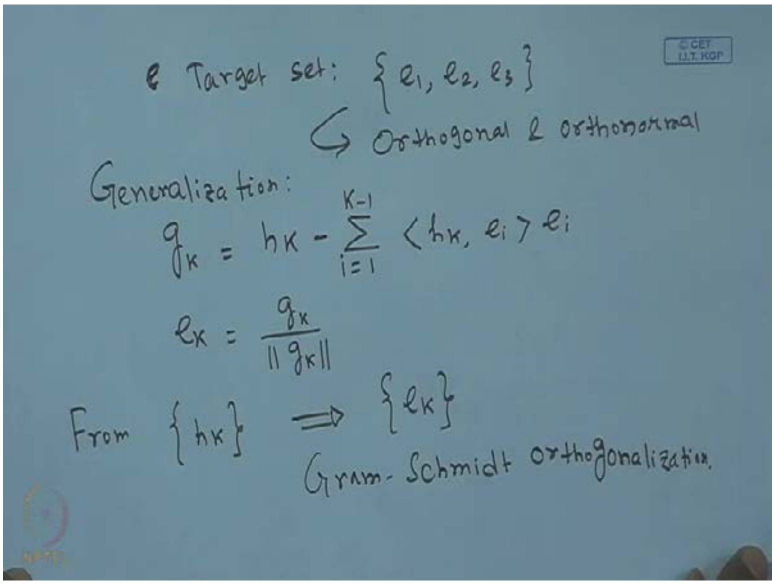

Now, we can say that we obtain the target set e, we have obtained e 1, e 2, e 3 from h 1, h 2 and h 3 and this set is basically orthogonal and orthonormal set. For kth space, this whole analysis can be extended and this can be generalized as. We will be obtained the kth vector as g of the target set as h k multiplied by summation of this i is equal to 1 to k minus 1 inner product of h k, e i multiplied by e i.

Using this generalized formula one can obtain keep on getting the vectors g 1, g 2, g 3, g 4, g 5, up to g k and then, make e k as orthonormal by defining this. So, you will be getting from h k set of independent vectors, we will be getting e k set of independent vectors which are orthogonal as well as orthonormal. So, this is the principle of Gram-Schmidt orthogonalization. So, using this technique, one can get a set of in deformed form of any set of independent vectors into an orthogonal and orthonormal set of vectors.

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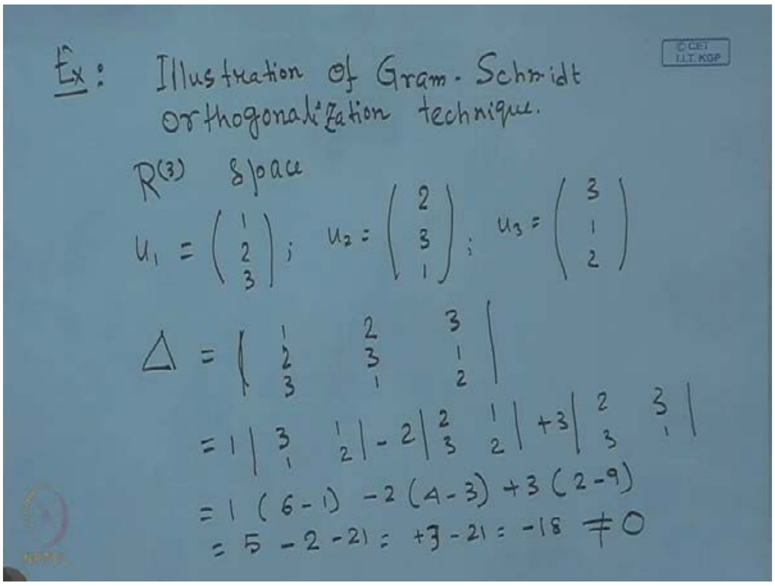

Next, we will take up an example to illustrate the Gram-Schmidt orthogonalization technique and the different calculations those are involved here. So, next example, we take to illustrate these techniques; so, this is nothing but illustration of Gram-Schmidt orthogonalization technique. We consider three-dimensional real space and you consider 3 vectors u 1 as 1 2 3; u 2 as 2 3 1; u 3 as 3 1 2 and we check whether these 3 vectors constitute an independent set of vectors or not.

In order to test that we evaluate the determinant forming by the elements of this vectors. So, it will be 1 2 3 2 3 1 3 1 2, so it is 3 into 3 determinant. Just open up this determinant, if you open up this determinant this becomes 1 multiplied by 3 1 1 2 minus 2, so this will be 2 3 1 2 plus 3 this will be 2 3 3 1 (Refer Slide Time: 15:59).

Next step do the internal calculations, so this will be 2 into 3, 6 minus 1 minus 2, 2 into 2 4 minus 3 plus 3 multiplied by 2 into 1 is 2 minus 3 into 3 is 9. So, it will be 6 minus 1 is 5 minus 1 into 2, this will be minus 7 into 3, so it will be minus 21. This will be minus 7 minus 21, it will be plus 7 minus 21, no, this will be 5 minus 2 is 3, 3 minus 21, so it will be minus 18 of course, this will be not equal to 0.

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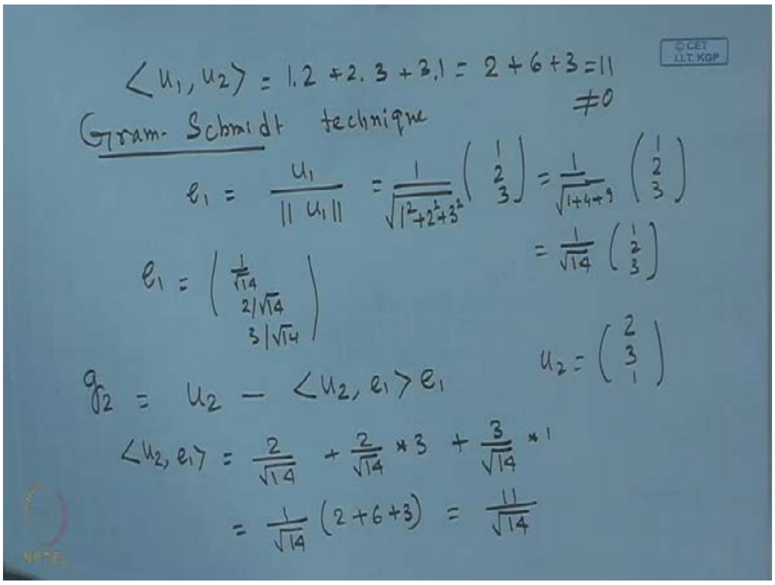

So, therefore, since the determinant is not equal to 0, the set constituted by u 1, u 2 and u 3 forms the independent set of vectors. Now, ofcourse, if you look into the values, if you take the inner product of these vectors, let us say, u 1 and u 2, the inner product will be 1 into 2 plus 2 into 3 plus 3 into 1. So, this becomes 2 plus 6 plus 3 is equal to 11; so, this is of course, not equal to 0; that means, although u 1, u 2, u 3 are independent to each other, but u 1 and u 2 and u 3 they do not form an orthogonal set of vectors.

So, now, we have to take request to the Gram-Schmidt orthogonalization technique and evaluate from u 1, u 2, u 3 set will be getting e 1, e 2, e 3 set such that e 1, e 2, e 3 will be mutually orthogonal and orthonormal. The first element we are targeting at is e 1; e 1 is nothing but u 1 divided by norm of u 1. So, u 1 is 1 2 3, so it will be 1 2 3 and norm of u 1 will be nothing but root over 1 square plus 2 square plus 3 square. It will be 1 over root over 1 plus 4 plus 9, 1 2 3. So, this will be 1 over root over 14, 1 2 3. These gives this u 1 is the first vector of our target set e. So, e 1 is nothing but 1 over root over 14 2 over root over 14 3 over root over 14.

Next, we go for the second vector of this set that will be given by g 2; g 2 if you remember this is nothing but, u 2 minus inner product of u 2 and e 1 multiplied by e 1. What is u 2? If you remember u 2 is nothing but 2 3 and 1. Let us first calculate this inner product between u 2 and e 1 as 1 by root over 14 into 2, so it will be 2 divided by root over 14 plus 2 divided by root over 14 into 3 plus 3 divided by root over 14 into 1. So, it will be, if you take root over 14 as common this becomes 2 plus 6 plus 3, so this becomes 11; so, 11 divided by root over 14. So, that is the inner product of u 2 and e 1.

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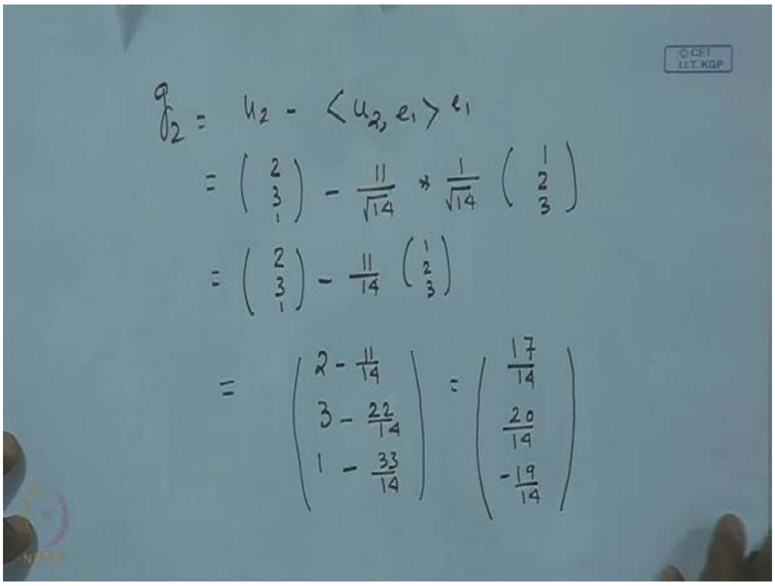

Now, we are in a position to formulate the value of the vector g 2. The g 2 now becomes u 2 minus inner product of u 2 and e 1 e 1. So, this becomes 2 3 1 minus 11 by root over 14 multiplied by e 1 and e 1 if you remember this is 1 over root 14 1 2 and 3. This becomes 2 3 1 minus 11 by 14 1 2 3. We are in a position to get the elements of the vectors g 2, this will be 2 minus 11 by 14, next will be 3 minus 2 into 11 by 14 that is 22 by 14, next will be 1 minus 11 by 14 into 3, so it will be 33 by 14.

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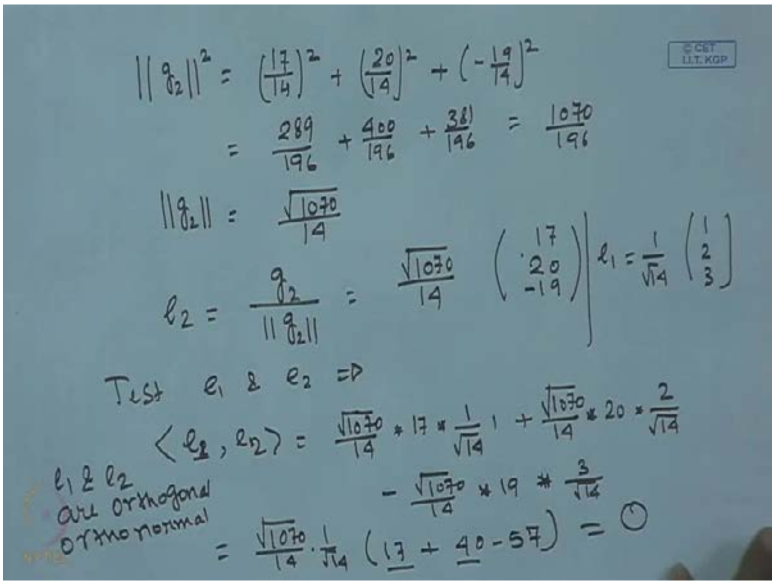

You can simplify this equation and this becomes 17 by 14 20 by 14 and minus 19 by 14. So, we get the vector g 2 and then we make it orthonormal; so, therefore, we make its norm has to be 1. So, we evaluate the norm of g 2 this becomes 17 by 14 square of that plus 20 by 14 square of that plus minus 19 by 14 square of that. These become 289 by 196 plus 400 by 196 plus 381 divided by 196. The whole thing becomes 1070 divided by 196 and norm of g 2 is now nothing but root over 1070 divided by 14. So, we are in a position to get the second element of the target set e 2 as g 2 divided by norm of g 2 and this will be root over 1070 divided by 14 17 20 minus 19. So, that gives the second element e 2 of our thing.

Now, we can test whether e 1 and e 2 are orthogonal to each other or not. So, it is sure that they are orthonormal. So, if you take the inner product of e 1 and e 2 will be, so this is e 2 and if you write e 1 just next to it, this becomes 1 over root over 14 1 2 and 3.

If you evaluate this one, this will be root over 1070 divided by 14 into 17 into 1 over root over 14 multiplied by 1 plus root over 1070 by 14 multiplied by 20 multiplied by 2 root over 1 by 14 minus root over 1070 divided by 14 multiplied by 19 multiplied by 3 divided by root over 14.

If you take root over 1070 by 14 and 1 by root 14 common, we will be getting 17 plus 40 minus 57, so 17 plus 40 is 57, 57 minus 57 is 0. So, these whole thing become 0; so, these become 0.

The inner product between e 1 and e 2 become 0; that means, e 1 and e 2 are orthogonal. Since, each of them is orthonormal they are orthonormal as well. So, therefore, these two elements e 1 and these two vectors e 1 and e 2 are the first two members of my target set e.

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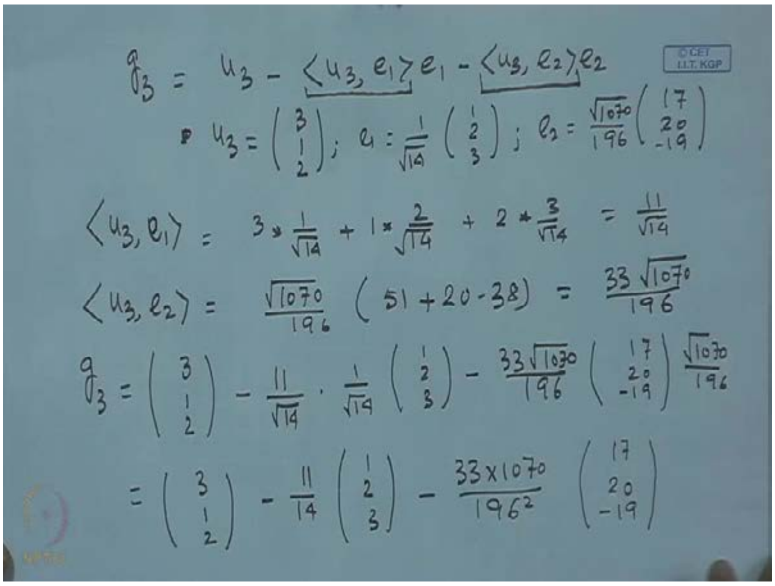

Next will be calculating the third vector g 3 and if you remember g 3 is nothing but u 3 minus inner product of u 3 and e 1 multiplied by e 1 minus inner product of u 3 and e 2 multiplied by e 2. So, just for the sake of, follow easiness to follow up, we just write down the values of these three vectors u 3 is 3 1 2, e 1 is 1 over root over 14 1 2 3 and e 2 is root over 1070 divided by 196 17 20 minus 19. We first evaluate the inner product of u 3 and e 1, next we evaluate the inner product of u 3 and e 2, so things becomes simplified later on.

So, inner product of u 3 and e 1 is nothing but 3 multiplied by 1 over root over 14 plus 1 multiplied by 2 over root over 14 plus 2 multiplied by 3 over root over 14. So, this becomes 11 by root over 14. And, inner product of u 3 and e 2 can similarly be calculated as, root over 1070 divided by 196 multiplied by 51 plus 20 minus 38. So, u 3 and e 2, so this multiplied by this, plus 1 multiplied by 1070 divided by 196 into 20 likewise, you will be getting this as 33 root over 1070 divided by 196.

We will be in a position to get g 3 now more accurately. So, g 3 will be u 3, u 3 is 3 1 2 multiplied by 11 by 14, this one, inner product between u 3 and e 1 11 by root over 14 multiplied by 1 over root over 14 1 2 and 3 minus inner product of u 3 and e 2, this will be 33 root over 1070 divided by 196 and this one will be 17 20 minus 19 multiplied by, it has root over 1070 divided by 196. So, this becomes 3 1 2 minus 11 by 14 1 2 3 minus 33 into 1070 divided by 196 square into 17 20 minus 19 (Refer Slide Time: 27:58).

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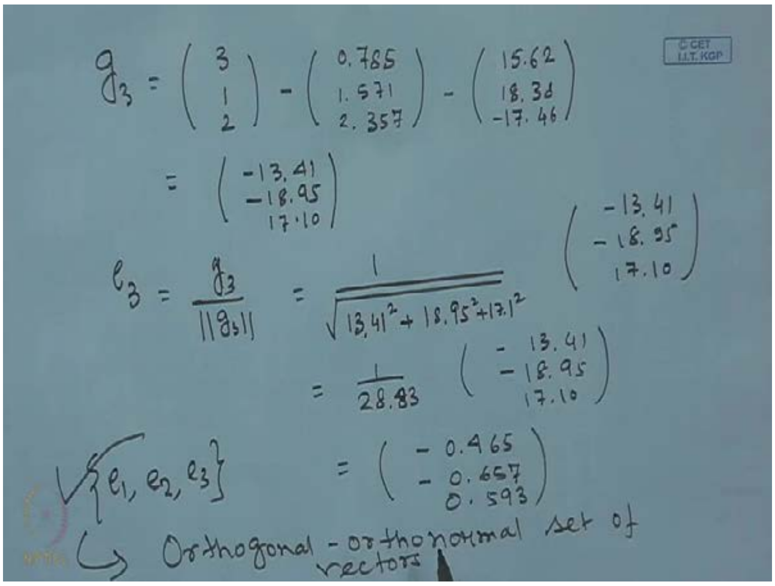

So, now, we should get into the decimals and simplify this equation. So, g 3 now becomes 3 1 2 minus 0.785 1.571 2.357 minus 15.62 18.38 minus 17.46. This becomes after simplification 13 minus 1.41 minus 18.95 17.10. So, that is the third vector g 3 which is orthogonal to each other with e 1 and e 2, but to make it orthonormal, we have to normalize g 3 by this formula g 3 divided by norm of g 3.

So, this will be 1 over root over 13.41 square, this minus minus will be gone, when the square is taken 18.95 square plus 17.1 square and this will be minus 13.41 minus 18.95 17.10 and after taking the square root this becomes 1 over 28.83 minus 13.41 minus 18.95 17.1. You will be getting as minus 0.465 minus 0.657 and this will be plus 0.593.

So, we get the vectors of the target set e 1, e 2 and e 3, where e 1 and e 2 are mutually orthogonal, e 2 and e 3 orthogonal, e 3 and e 1 orthogonal and each of them will be having a norm 1; that means, we are getting an orthogonal - orthonormal set of vectors, out of independent vectors u 1, u 2 and u 3. So, this gives the demonstration how Gram-Schmidt orthogonizational technique is utilized in order to make the basis and vectors into orthogonal and orthonormal set of vectors.

Next, we go to the topic of contraction mapping and contraction mapping is a very important mathematical technique and may be, well utilized by the chemical engineers to analyze the unique steady state or unique solution to a problem. So, therefore, this is very important technique, all the chemical engineering processes are depending on basically the quality of the processes will be evaluated, what is the product quality you are going to get.

Suppose, we are having a process there are certain inputs into the system and the system gives some outputs. Now, the quality of the output becomes very, very important for example, if you talk about a polymerization reaction, there will be a polymerization reactor or the polymerization reaction is going on; we are going to have certain reactants getting into the systems may be, monomers and some of the co-polymers or some of the catalyst may be getting into the system and what is the output of the system? From the output, we are going to get polymers of various grades.

Now, grading of these polymers the quality of the polymers are extremely important; for example, these polymers will be having certain properties; the importance on the utility of this products will be evaluated by the properties.

For example, the polymer properties are evaluated in terms of certain physical properties; for example, milt flow index that is directly related to the viscosity of the product, milt flow index stress exponent things like this. Now, all this properties have to be evaluated and generally, these properties are desirable within a narrow range. For example, if we going to get milt flow index in the range of 8.5 to 8.8 that will be grade 1 polymer.

If we are going to get a range of this particular property between 0.90 - 0.95 will give me another grade of polymers and each of such products will be having its specific utility and use. Now, if we cannot control these qualities of the product, then the whole batch will be spoiled and you will be wasting huge amount of man power energy and material and money.

Of course, in order to get that, we would like to operate the whole system in a steady state and that steady state has to be unique steady state, there may be a mild fluctuation in the real time operation, but the steady state has to be unique one. We should not land up with a multiple steady state, where in one case we are going to get a product quality of specificity between a range r 1. In another steady still going to get another product quality in the range r 2, where r 1 is desirable and r 2 is not desirable.

So, therefore, the identification of the operating conditions which will make your system having a unique steady state is extremely important for the chemical engineers. There exists a fixed set of operating conditions which will give me a unique steady state or a unique fixed point; we call it mathematically in a chemical engineering operation.

Determination of steady state and whether that the steady state is unique steady state and what are the conditions of the operating parameters that will ensure that unique steady state is very important for the chemical engineers to control the chemical engineering processes. So, contraction mapping is one such techniques which mathematically can tell you what will be the condition of the operating parameters, such that you are going to learn the steady state and the steady stage is ensure to be unique steady state.

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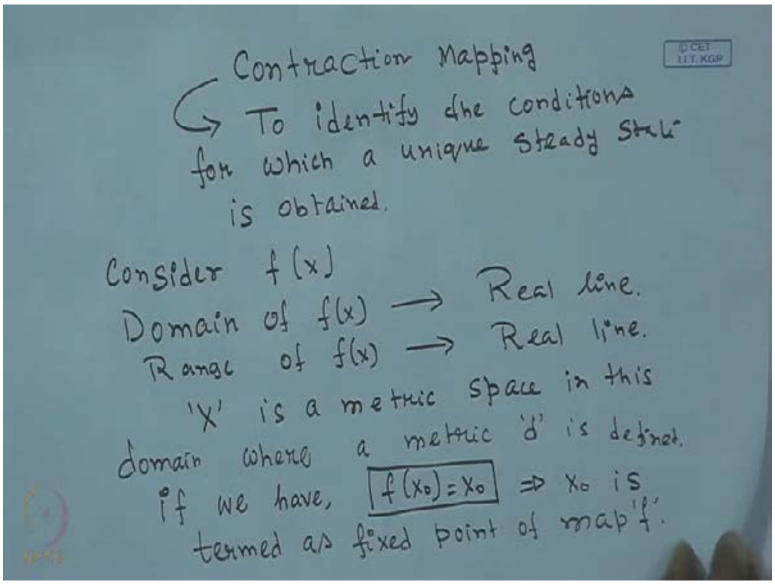

We start with the contraction mapping, so the utility of this technique is to identify the conditions for which a unique steady state is obtained. What we will do? We will have the mathematical formulation of this contraction mapping and we look into the theory of this development and then, we will be taking of a couple of examples maybe 4, 5 examples of different chemical engineering system to demonstrate the use of contraction mapping in order to identify the conditions for having a unique steady state.

Consider, let us look into the mathematical development and the mathematical analysis involved behind this contraction mapping technique. Consider the function f x and domain of f x is a real line. This is a real line, so we are working in real domain and range of f x is also a real line.

Now, x is a metric space in this domain, where a metric d is defined. Now, if this is the system then, if we have a relationship in this form f x naught is equal to x naught. If we can mathematically describe a chemical engineering system in this form, f x naught is equal to x naught then, x naught is termed as a fixed point of map f. If in your chemical engineering system, we write down the mathematical formulation to mathematically express this system and if it is ultimately in this form, x naught is equal to f x naught then x naught is termed as a fixed point to the map f.

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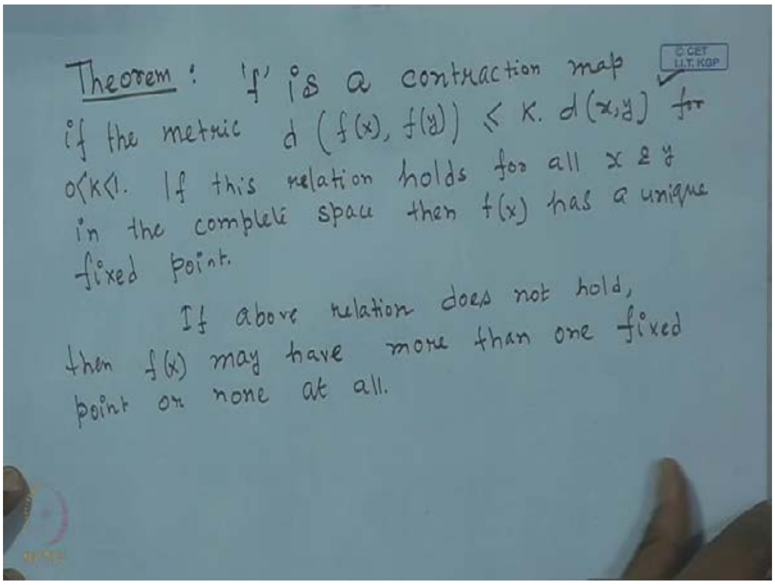

Next, we look into the theorem of contraction mapping. The theorem goes like this, f is a contraction map, if the metric d of f x and f y is less than k times metric between x and y for k lying between 0 to 1. We should call the map f as a contraction map if the metric between f x and f y is less than equal to k times metric between x and y, where k is a fraction then, we call this, if this relationship is obeyed then this map f is called a contraction map.

Now, next is if this relation holds for all x and y in the complete space then f x has a unique fixed point. This is the definition of contraction map, if metric between f x and f y is less than k of k times metric between x and y, where k is a fraction. If this relations hold for every x and y in the complete space, then f x has a unique steady state.

Now, what happens if this relation does not hold? If the above relation does not hold then f x may have more than, not unique, more than one fixed point or none at all. If this relation does not hold that does not mean that it will be a having more than one fixed point, it may not have any fixed point at all, but if this relation holds it is ensured that you will be having a unique fixed point.

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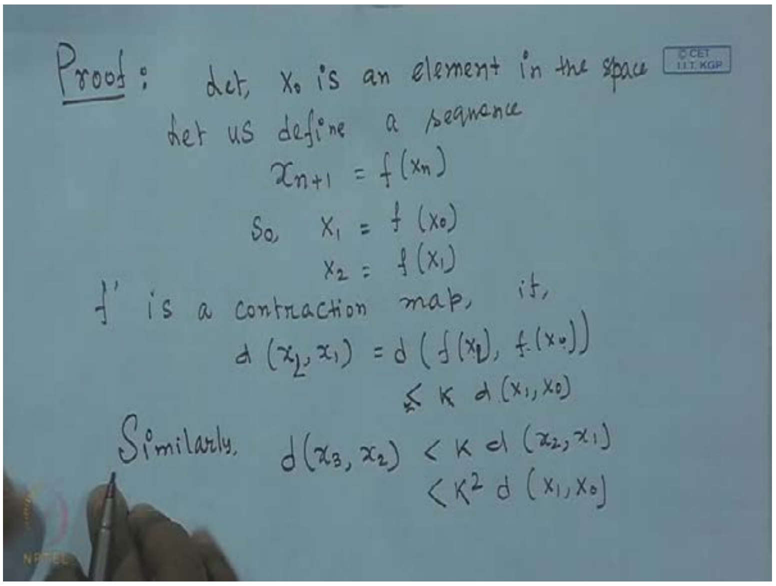

Let us go into the proof of this theorem. The proof goes like this, let, x naught is an element in the space and we define a sequence. Let us define a sequence, such that x n plus 1 is equal to f of x n. Therefore, x 1 is nothing but f of x naught, x 2 is nothing but f of X 1 likewise.

Now, f is a contraction map, if metric between x 2 and x 1 which is nothing but x 1 is nothing but f of x 1 metric between f of x 1 and metric between x 2 and x 1, so x 2 will be nothing but f of x 1 and x 1 is nothing but f of x naught is less than equal to k times, it is basically less than k times metric between x 1 x 2.

We are assuming that f is a contraction map in that case, d of metric between x 2 and x 1 should be nothing but identically equal to a metric between x 2 is nothing but f of x 1 and x 1 is nothing but f of x naught. But, if f is a contraction map then this relationship must be holding good; that is metric between f of x 1 and f of x naught should be less than k times metric between x 1 and x naught.

Similarly, we can have metric between x 3 and x 2 should be less than k times metric between x 2 and x 1 identical logic, so metric between x 2 and x 1 is less than k times metric between x 1 and x 2. By combining this two, we can write this will be nothing but k square d times metric between x 1 and x naught.

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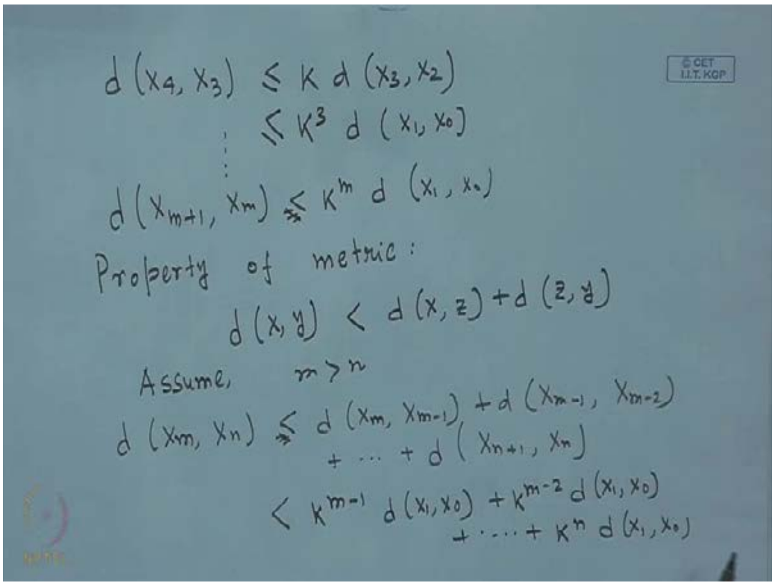

With the identical logic, we can go to the next step and write metric between x 4 and x 3 should be less than k times metric between x 3 and x 2. We have already proved that metric between x 3 and x 2 should be less than k square metric between x 1 and x naught. So, this will be less than k cube metric between x 1 and x naught. Therefore, we can continue like this and we can get a generalized equation, metric between x m plus 1 and x m should be less than k to the power m d metric between x 1 and x 0.

Now, we look into the triangle in equality of the metric property. Go to the property of metric, this property says that metric between x and y should be less than metric between x and z plus metric between z and y. Now, we assume m much greater than n, using this triangle rule of metric, we can write down metric between x m and x n should be less than equal to, less than metric between x m x m minus 1 plus metric between x m minus 1 x m minus 2 plus dot dot up to metric between x n plus 1 and x n.

We have already found out that metric between x m and x m minus 1 by this relationship, it will be just we change the indices. So, it becomes k to the power m minus 1 metric between x 1 and x 0, this will be nothing but k to the power m minus 2 metric between x 1, x 0 up to k to the power n metric between x 1 and x 0.

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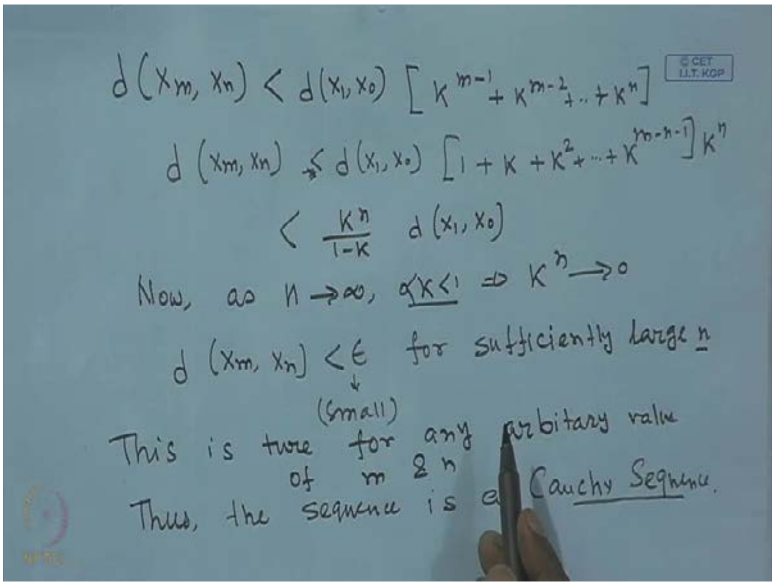

In a sense, we will be getting a series type of equation out of this and we further proceed and simplify this equation. So, metric between x m and x n can now be written as metric between x 1 and x 0 that is a scalar, so it has to be taken common and we can write it down as k to the power m minus 1 plus k to the power m minus 2 up to k to the power n, so this becomes a series. So, metric between x m and x n can be written as metric between x 1 and x 0 and this series can now be, we can take k to the power n as common, this becomes 1 plus k plus k square plus k to the power m minus n minus 1, we take k to the power n as common. So, this becomes k to the power n 1 over 1 by minus k d to the power metric between x 1 and x 0.

Now, as n increases, n goes up to infinity and k being a fraction, k is less than 1, so k to the power n goes to 0 as k lying between 0 and 1, it is a fraction, so as n tends to infinity k to the power n tends to 0. Therefore, metric between x m and x n is much less than epsilon for sufficiently for epsilon is a small quantity, quite small for sufficiently large n. Since, it is true, this relationship is true for any arbitrary value of m and n. The sequence we are talking about is a Cauchy sequence. Thus, the sequence is a Cauchy sequence and x n converges, since, it is a Cauchy sequence the value will be, so the sequence is a converging sequence and it will be converging to a point and that point is a fixed point.

We have already proved that using contraction mapping that for the function f metric between f x and f x 1 and f x 2, f x m and f x n for sufficiently large values of m and n if it is less than k times metric between x 1 and x 0, it will be converging to a fixed point x naught and that proves the contraction mapping.

Using contraction mapping, how one will be getting a converging sequence; next, the whole sequence will be convert to a fixed point, but next we will be proving that this fixed point is a unique fixed point. Once, we prove that then whole proof will be complete then you can go to a proper appropriate chemical engineering application. So that I will take up in the next class, thank you very much for your kind attention.