Statistics for Experimentalists
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Lecture – 47
Experimental Design Strategies - B

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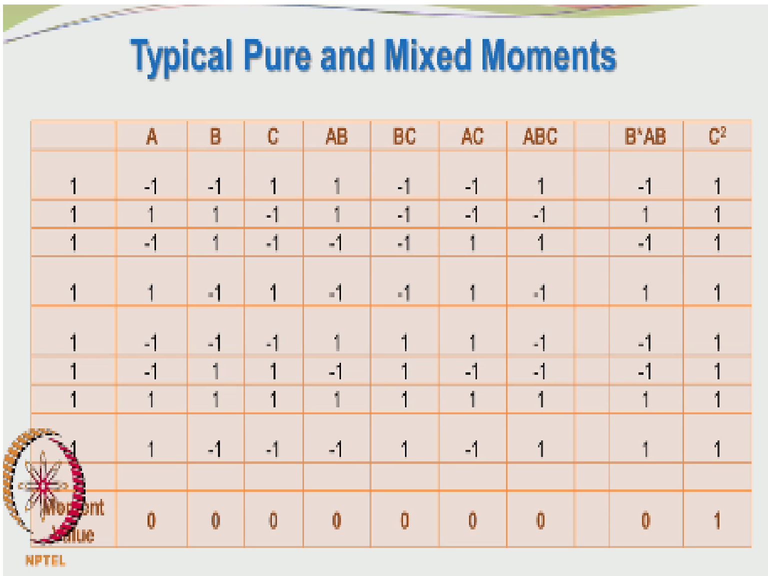

	A	B	C	AB	BC	AC	ABC		B*AB	C²
1	-1	-1	1	1	-1	-1	1		-1	1
1	1	1	-1	1	-1	-1	-1		1	1
1	-1	1	-1	-1	-1	1	1		-1	1
1	1	-1	1	-1	-1	1	-1		1	1
1	-1	-1	-1	1	1	1	-1		-1	1
1	-1	1	1	-1	1	-1	-1		-1	1
1	1	1	1	1	1	1	1		1	1
1	1	-1	-1	-1	1	-1	1		1	1
Moment Value	0	0	0	0	0	0	0		0	1

Let us now look at a saturated 2 power 3 factorial design X matrix and so, in addition to the intercept, we also find the ABC, AB, BC, AC and ABC that would be a 1 + 7, 8. So, all the 8 settings are being used up to determine 8 parameters and when you look at the A column, you are having -1, +1 is an orthogonal design and so the number of -1 should be = the number of +1 and so the total will be = 0.

Similarly, for B, you will again have a total of 0 and so on for see C as well. If you look at AB again, you are going to have a combination of + 1's and – 1's in equal numbers and so it will become = 0 and when you look at ABC also, we are going to have as 0, so we can see that the first order moments are 0 because we are summing the elements in the X matrix column wise for a given X.

In this case, Xi will be = A or i is = A, if you want to put it that way, so the first moments are all 0 and this is the second mixed moment because A is different from B, again that is = 0 so, is BC and AC and when you are looking at the third moment, which is also mixed because you are having A and B, which is different and also B and C are different, A and C are different and so when you look at the sum, it is again = 0.

So, we can see that the third mixed moment is = 0 and even AB squared even though, you are having the B squared term, you are having A to the power of 1 and hence you are having a mixed moment here and that would be a third mixed moment, which is = 0. Only, when you come to C square, all the elements become 1 and when you total it up, you are going to get 8 but anyway you are dividing it by the total design size, which is again 8.

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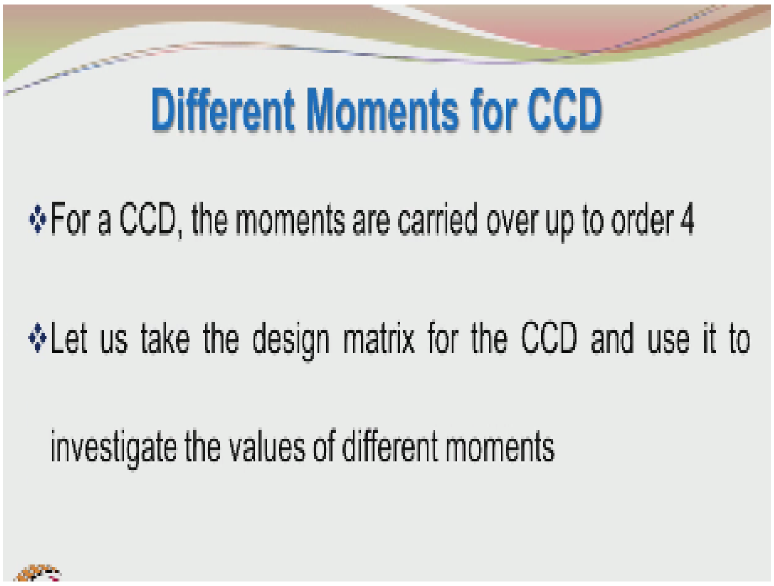

And so, 8/8 will give you 1, so this is the way in which the pure and mixed moments are computed for various designs. Now, when you look at a central composite design, which are now having center points and also the axial points, the moments are carried over up to order 4, so we will take the design matrix for the central composite design and use it to investigate the values of the different moments.

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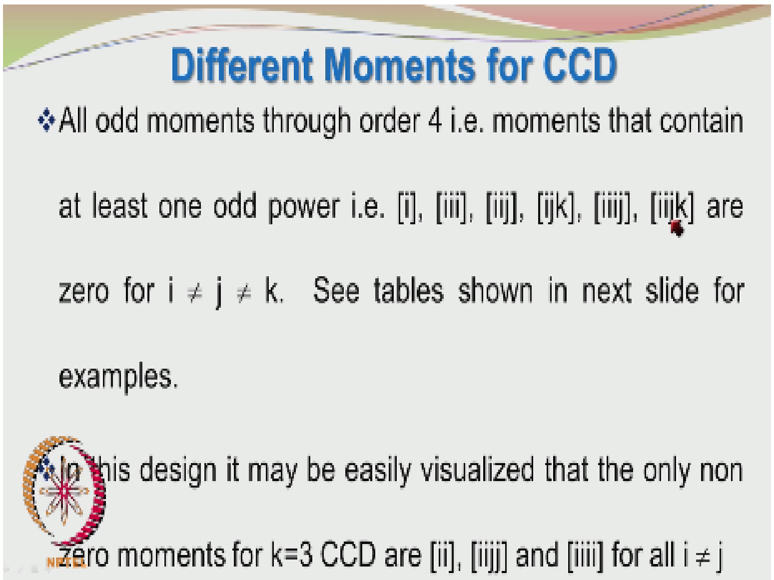

So, all odd moments through order 4 that is the moments that contain at least 1 odd power, so i; i to the power of 1, i cube, i to the power of 3, i square j, i to the power of 2 and j to the power of 1, so it is an odd moment or a mixed moment, ijk; all of them are different and all of them have odd powers, i cube j, so 3 is also odd and the 1 is also odd, the 3 is exponent for i and 1 is the exponent for j, both of them are odd numbers.

And so we can call them as odd moments or mixed moments and then we also have i square jk are 0 for i not = j, not = k, so the tables chart shown next will illustrate this concept. Also, when are we going to have the nonzero moments? It appears that many of the moments are 0, are there any moments which are non-zero and for the central composite design involving 3 factors; the nonzero moments are; for k is =3, corresponding to i square, i square j squared, i to the power of 4 for all i not = j.

So, these are the cases where the moments will not be = 0 but will the moments be = 1, again this is a very interesting question because N is the size of the run, so N would be the number of experimental settings and for a central composite design, it can be shown for 3 factors, you have 8 factorial points; 2 8 3, 6 axial point, so 8 + 6 that makes it 14 and then you have 14 + nc center points.

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But what would be the values taken by the nonzero moments such as i square, i square j square and i to the power of 4, we will have to compute them. Let us look at the table, so let us look at the moments table for 2 power 3 design with 6 center points, 8 factorial points that would be again 6 axial points, a total of 20 points.

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	[i]	[ij]	[iii]	[iij]	[ijk]	[iiij]	[iijk]
BC	C	A*B	C^3	(A^2)*B	ABC	(B^3)*A	(C^2)*A*B
0	0	0	0	0	0	0	0
-1	1	-1	1	-1	-1	-1	-1
-1	-1	-1	-1	1	1	-1	-1
0	-1.682	0	-4.757	0	0	0	0
1	-1	-1	-1	-1	1	-1	-1
-1	1	1	1	-1	1	1	1
0	1.682	0	4.757	0	0	0	0
0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
1	1	1	1	1	1	1	1
0	0	0	0	0	0	0	0
-1	-1	1	-1	1	-1	1	1
1	-1	1	-1	-1	-1	1	1
0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
[illegible]	1	-1	1	1	-1	-1	-1
0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
[illegible]	0	0	0	0	0	0	0
Total:	0	0	0	0	0	0	0

So, this is 20; 1,2, 3, 4, 5, 6, so this entire column comprises of 20 elements, this is for A and you can see that in addition to the -1 and -1 + 1 + 1 – 1 – 1, these correspond to the factorial points. So, the number of + 1's and the number of – 1's are matching, so that is fine and this -1.682 and +1.682 refer to the axial points. Similarly, B also has such share of equal number of -1 and +1 points and then it also has 1.682 and -1.682, which correspond to the axial points.

Same way, we can do for C, now if I add up the elements in the A column that will correspond to the first moment and that would be = 0, so would be the first moment corresponding to B and C but if I look at A square, I am going to get 1, 1, 1, 1, so i will get 1, 2, 3, 4, 5, 6, 7, 8; 8 1's and then i am also going to get square of – 1.682 and again square of +1.682, which turns out to be 2.828 and 2.828.

So, when I total the elements of the A square column vector, I am not going to get N as I get for the pure factorial case because now, the central composite design we have added the axial points, so the axial point coordinates also will contribute to the moment, which is not vanishing. If I look at the A squared vector or the A squared column, I am seeing elements, which are all 0 or only positive.

When I add up the elements, I am not going to get a value of N, where N is the design size, here N is = 20, I will get a value different from N because we have 8 ones that would be 8 and then you also have 2.828, 2 times, which is approximately 5.656, so 13.5656. So, that value is not = N, which is 20. I am just illustrating the difference between the central composite design and the regular factorial design.

Similarly, for B squared, you have again a pure second order moment and when you total it up, the value will be same as that of A square. Similarly, for C square, when you however look at the second order mixed moments or the odd moments comprising of AB or AC, where A is different from B and A is different from C, we see that the total adds up to 0. So, the moment values for the second order mixed moments are 0.

We can go on for BC, C, AB, C cube, A squared B and ABC, B cube A, C squared AB, so as long as you have odd moments, the moments are carried over up to order 4, we can see as long as there are at least 1 different term in the product. For example, in C squared AB, AB and C square are different and when you look at AB cube, A and B are different, A squared B, A and B are different, all the cases the moment value becomes 0.

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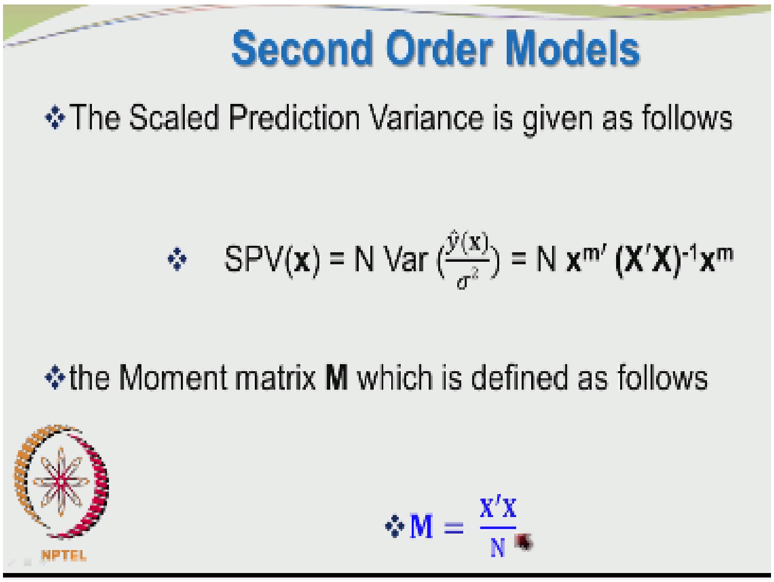

When you add up the elements in the column, they all become 0 here. So, now we are going to the second order models, the scaled prediction variance is normalizing the design size by multiplying by N and removing the variance effect by dividing by sigma squared and so we simply get N * xm prime X prime X inverse xm, we saw that xm prime is the coordinate point in the experimental design space expanded into the model space.

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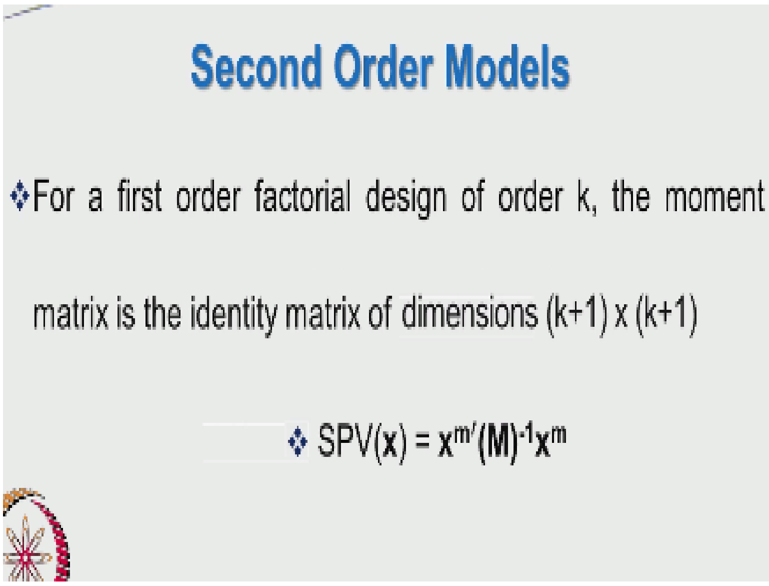

So, that xm reflects the model we have chosen to represent the process, when we have also seen that the moment matrix is given by x prime x/ N. So, for a first order factorial design of order k, the moment matrix is the identity matrix of order k + 1/ k +1 that can be easily shown and we have also shown it a few times earlier, so we get using the definition for M; M as x prime x/ N, so x prime x inverse would be substituted in terms of M and N.

The N cancels out and then we get M inverse here, so this derivation is pretty straightforward, if you want you can try it out. So, what we are trying to prove here is the scaled prediction variance at a point X in the experimental design space depends upon the moment matrix and the scaled prediction variance of X would be XM prime M inverse and XM and you just put the identity matrix here, instead of M inverse, so identity matrix inverse is also an identity matrix.

So, you will have identity matrix here and then it will be each element multiplied with itself in the xm Prime and xm, so this can be easily verified in our earlier lecture on orthogonal design concepts, we did calculate the scaled prediction variance. The scaled prediction variance we showed in the orthogonal design as 1 + square of the distance of the coordinate from the experimental design center, you may want to verify that.

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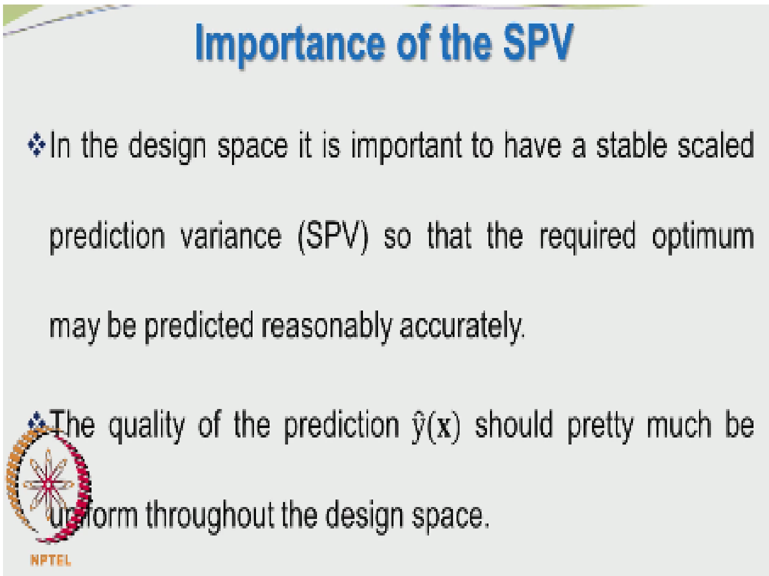

So, what is the importance of the scaled prediction variance, the design space? It is important to have a stable scaled prediction variance, if the stable nature of these SPV is violated, then you will have shooting up of the variance at some locations in the experimental design space and the model predictions can be considered to be reliable no longer. So, another thing is the quality of the Y hat of X should be as uniform as possible throughout the design space.

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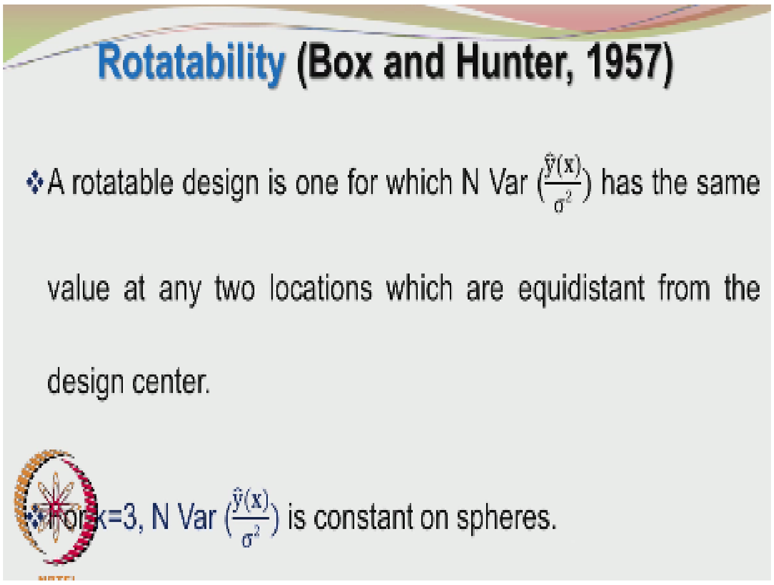

You cannot have certain pockets in the experimental design space, where the scaled prediction variance is hitting the roof. Now, let us look at the concept of rotatability, this was defined by Box and Hunter in 1957. A rotatable design is one for which N into variance y hat of x/ sigma squared, which is nothing but the scaled prediction variance has the same value at any 2 locations, which are equidistant from the design center.

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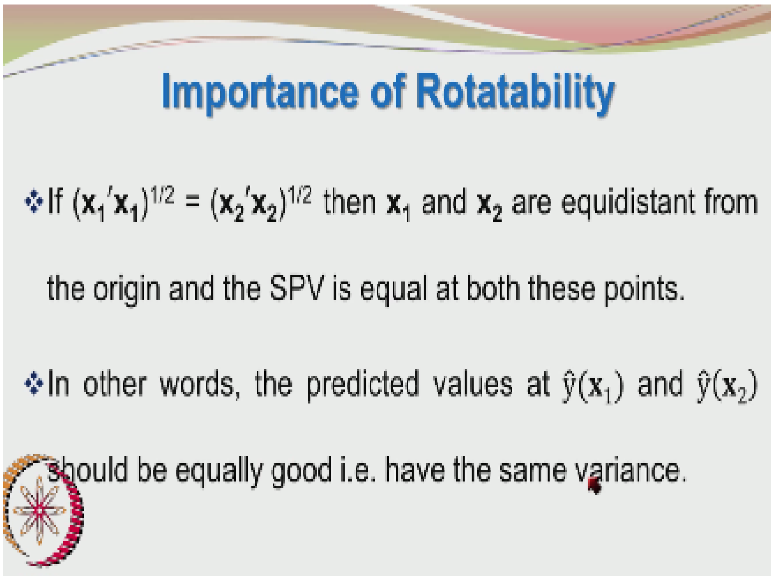

And for k is = 3, N * variance y hat of x/ sigma squared is constant on spheres because any point on the sphere would be equidistant from the center. So, let us take 2 points in the experimental design space; x1 and x2, if you have x1 prime x1 to the power of 1/2 is = x2 prime* x2 to the power of 1/2, then x1 and x2 are said to be equidistant from the origin and the scaled prediction variance is equal at both these points.

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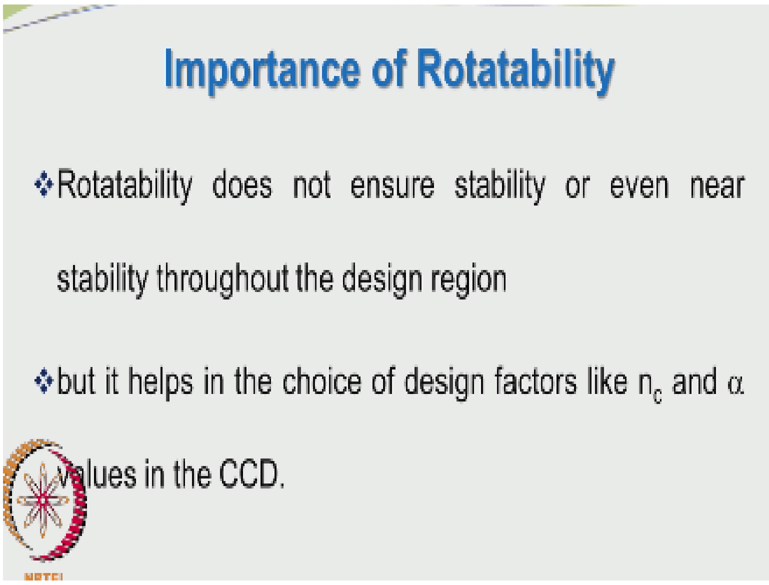

In other words, the predicted values at Y hat x1 and y hat x2 should be equally good that is have the same variance and just because the design is rotatable, it does not mean that the SPV is stable everywhere in the design space but the concept of rotatability also helps us to find the number of center points and also the coordinates of the axial points in the central composite design.

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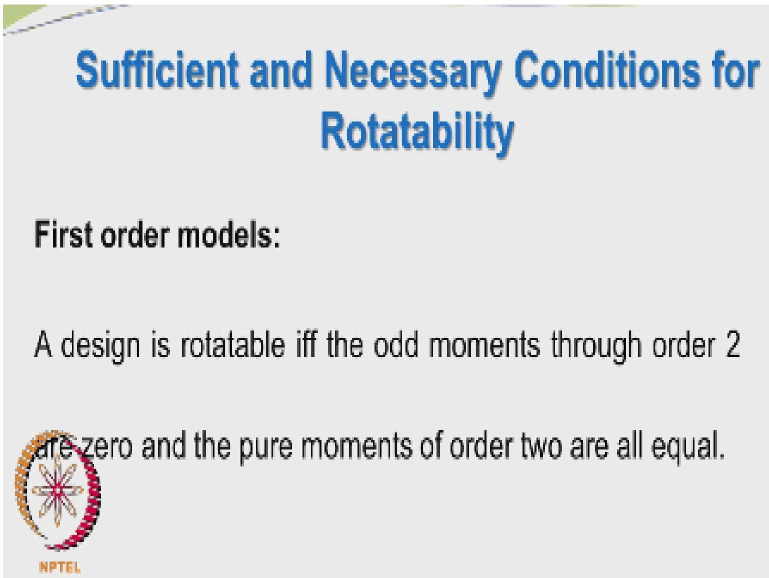

So, now if you look at the first order models, a design is said to be rotatable if and only if the odd moments through order 2 or 0 and the pure moments of order 2 are all equal.

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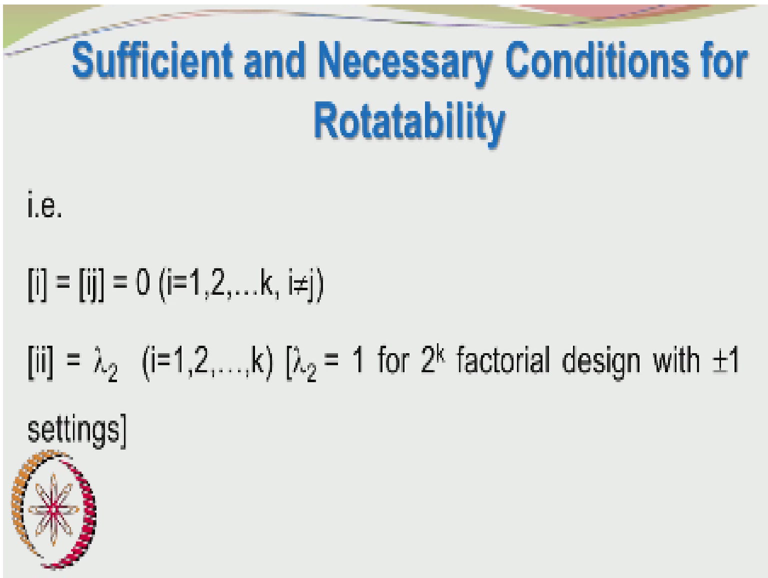

So, you have i is = ij is = 0, this can be easily verified for i is = 1, 2 so, 1 to k and i is not = j and then you also have i squared is = lambda 2, where lambda 2 is =1 for 2 power k factorial design with 1 -; + or – 1 settings. So, we are looking at the necessary and sufficient conditions for rotatability, we are discussing a first order design and in the first order design for rotatable conditions to exist, the first order moment as well as the second order odd moments or mixed moments should b = 0.

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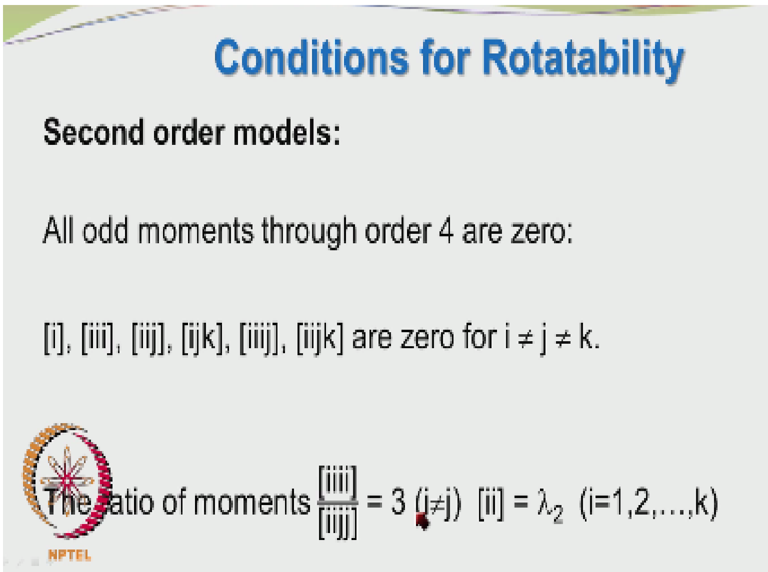

That means i is = ij is = 0 for i not = j, i squared is = lambda 2, where lambda 2 is a constant and it is not = 0 and for a 2 power k factorial design alone with plus or minus 1 settings lambda 2 is =1, this also we have seen previously. Again, looking at conditions; more conditions for rotatability for second order models, this is very important, all the odd moments through order 4 or 0.

And there is a difference between the mixed moment and the odd moments, if you have i squared j squared, they are considered to be mixed moments because i is not = j. On another hand, you are looking at the power; the power is 2 for i as less j, so you cannot call it an odd moment but it is a mixed moment but if you have i cube j, then the power of i is = 3 and the power of j is =1.

And so here you have odd moments, now when you are looking at odd moments through order 4 or 0, you have ii cube i square j, j is having a power of 1, ijk all the i, j and k are having powers of 1, i cube j, i squared jk or 0 for i not = j not = k and very interestingly, the ratio of the moments i power 4/ i square j square is = 3 and i squared is = lambda 2, so this is a very interesting condition; i power 4/ i square j square is = 3, for a rotatable design.

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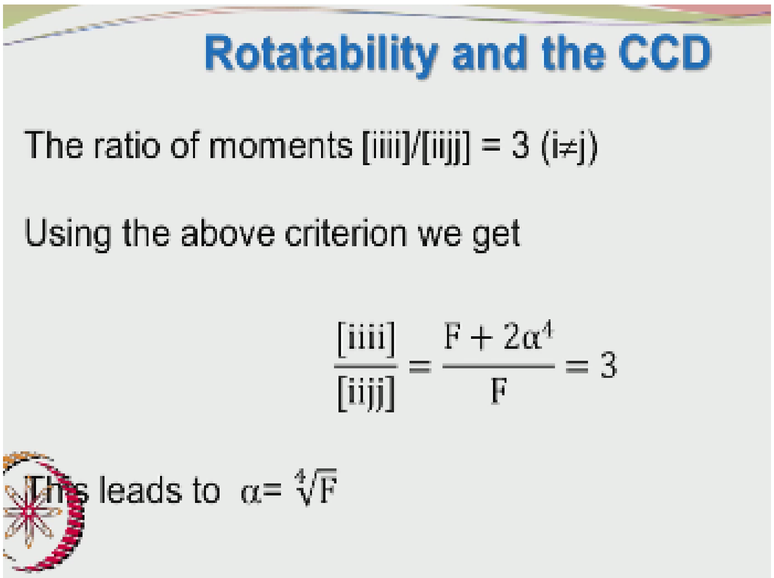

And so, when you look at i power 4, you will have the elements all 0 or positive, you would not have any negative values, you will have 0, 1 and then you will also have the axial points to the power of 4. So, for the factorial points they will all be 1, so the -1's will be converted into +1's, so they will all remain as 1's, 0's will of course be 0's, so when you total them up that will be equal to that total number of factorial points.

And then you are going to have to 2 alpha to the power of 4 because the axial points for each column would be + alpha and – alpha, when they are taken to the power of 4, it will become alpha to the power of 4 and alpha to the power of 4, so it will be 2 alpha to the power of 4 and so the 4th order pure moments would be giving a total of F + 2 alpha to the power of 4, whereas i squared j squared, it can be shown very easily will give you only F that is very interesting.

The 4th order mixed moments, i square j square is independent of the alpha term, whereas the pure 4th order moment is having the alpha term in it. So, the ratio of these 2; i to the power of 4/ i square j square moments is =3, for a rotatable design and here it can be easily shown that from this relation, we are going to have 3 F – F, which is 2F, so F is = alpha to the power of 4 or alpha is = 4th root of F.

And so, if you want your central composite design to be rotatable adopting these criteria helps you to find the value of alpha, this is what I have been telling about early in the lecture, we will has to; how the alpha values are going to be set. If you want a rotatable design, so using these criteria, we set the value of alpha as the 4th root of F, where F is the factorial number of points okay.

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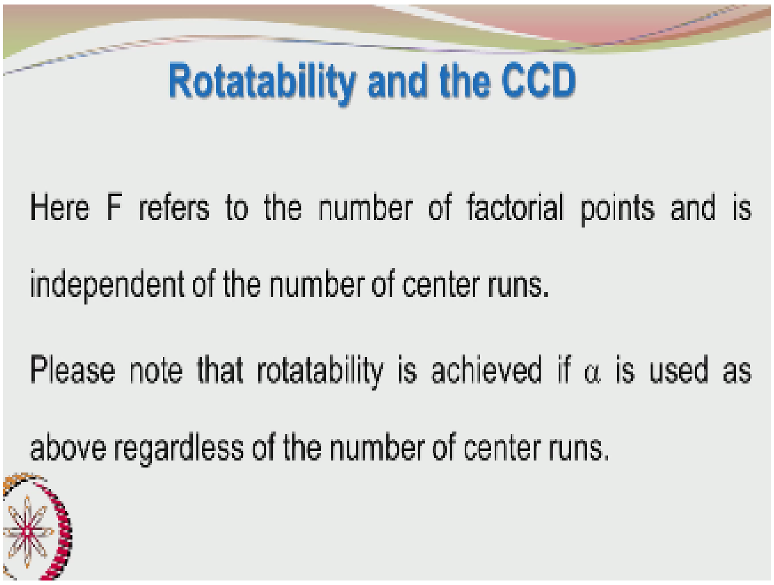

F is not the number of factors but the total number of factorial points, for 2 power 2 design, F would be = 2 power 2, which is 4, for a 2 power 3 factorial design, F would be = 8. So, F refers to the number of factorial points and is independent of the number of center runs, again you can see that the alpha value which is recommended to meet the condition of rotatability is independent upon; independent of the number of center runs.

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Ones	A	B	C	A²	B²
1	0	0	0	0	0
1	1	-1	1	1	1
1	-1	1	-1	1	1
1	0	0	-1.68179	0	0
1	1	-1	-1	1	1
1	-1	-1	1	1	1
1	0	0	1.68179	0	0
1	-1.68179	0	0	2.82843	0
1	0	0	0	0	0
1	1	1	1	1	1
1	1.68179	0	0	2.82843	0
1	1	1	-1	1	1
1	-1	-1	-1	1	1
1	0	0	0	0	0
1	0	1.68179	0	0	2.82843
1	0	0	0	0	0
1	-1	1	1	1	1
[illegible]	0	-1.68179	0	0	2.82843
[illegible]	0	0	0	0	0
[illegible]	0	0	0	0	0
20					

Please note that the rotatability is achieved, if alpha is used as above regardless of the number of center runs. Let us now look at the 2 power 3 central composite design, we are having 20 runs. How did the 20 runs come about? We have 8 factorial points 2 power 3 factorial points which will be 8 and then you have also 6 axial points, they are located at -1.682, +1.682 and that would be 6.

So, because you are having 3 axis and so each axis has 2 axial points, so you have 6 axial points totally, 8 + 6 is 14 and then you also have 6 repeats, the repeats are not located in one group, you can see that this design has been randomized and so you are having the center points at different locations, this is one center point, that is one, this is the second center point because all the coordinates are 0, 0, 0, 0 that would be 2, so this is 3 and this is 4, 6 and 6.

So, we have 6 center points and you can see that the A square will not vanish either the terms are 0 or positive but for A, B and C, you have equal number of negative and positive values and so the total would be = 0, A square and B squared are not going to be 0, A square is -1.68 is square is 2.83, so these calculations are pretty straightforward, so I would not be discussing them any further.

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Ones	AB	AC	BC	[iiii] C⁴	[iijj] BBCC
1	0	0	0	0	0
1	-1	1	-1	1	1
1	-1	1	-1	1	1
1	0	0	0	8	0
1	-1	-1	1	1	1
1	1	-1	-1	1	1
1	0	0	0	8	0
1	0	0	0	0	0
1	0	0	0	0	0
1	1	1	1	1	1
1	0	0	0	0	0
1	1	-1	-1	1	1
1	1	1	1	1	1
1	0	0	0	0	0
1	0	0	0	0	0
1	0	0	0	0	0
1	-1	-1	1	1	1
1	0	0	0	0	0
1	0	0	0	0	0
1	0	0	0	0	0
20	SUM = 0	SUM = 0	SUM = 0	SUM = 24	SUM = 8

But when you look at the other elements, we are having the 4th order pure moment, C power 4, when you total it, it adds up to 24, interestingly the axial point has become 8, you can see that the axial point has become 8, so what is 1.68179. According to the conditions of rotatability, alpha is = 4th root of F, where F is the number of factorial points. So, the 4th root of 8 gives you 1.68179, if the 4th root of 8 is 1.68179, the 4th power of 68179 will be = 8.

And that is the reason why for C power for 4 column, we are getting 8 here and when you total it up, it adds up to a nice 24 and when you look at the 4th order mixed moments i square j square, the sum is equal to 8 because you are going to have B square and C square and you are not having the contribution from the axial point because the axial point in the B column is located at a different place than the axial point in the C column.

This is very easy to verify, here the axial points are here corresponding to the location of the axial point in the B column, the corresponding values are both 0, the axial point in the C column, yeah, I was pointing with the wrong column, this is the axial point in the B column and corresponding to that the values are 0, okay and the axial points in the C column are located at points, where the corresponding points in the B column are both 0.

So, you are having 0. 0 and then you are having these 2 and you are having these 2 and then you are having 0, 0 here. So, when you when you do B square, this term will of course be positive; both will be positive but when I am doing B square C squared, you can see that it will become 1.68179 squared * 0 square, which is 0, so that is why the B square C squared has zeros even at locations corresponding to the axial points for the B and C columns.

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Values of α for rotatable CCD

k	F	N	$\alpha = \sqrt[4]{F}$
2	4	$4+4+n_c$	1.414
3	8	$8+6+n_c$	1.682
4	16	$16+8+n_c$	2.000
5	32	$32+10+n_c$	2.378

Anyway, if you take the ratio of C to the power of 4 and B square, C square, if you take the ratio of C power 4 to B square C square, you get 24/8, which is = 3. Now, let us see the values of alpha for a rotatable central composite design, for k is = 2 and 4 factorial points, the total number of design points would be 4 + 4 + nc and alpha is = 4th root of 4, which is 1.414, 4th power of 4 would be root 2 and that is why you are getting 1.414.

And for k is = 3, it can be easily shown just now, we saw that the alpha is 1.682, for the factorial; for design involving 4 factors, k is =4, we have F is = 16 and alpha is coming to a whole 2 and when you look at 5 factors, the number of factorial points would be 2 power 5, which is 32, the total number of points would be 32 + 10 + nc and alpha is coming out to be 2.378.

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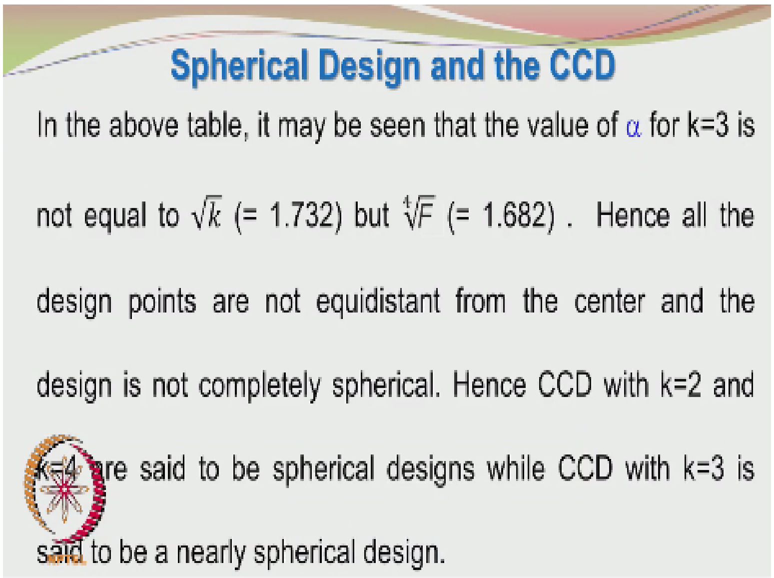

Now, let us see whether the design is spherical, for a spherical design, you want the points to be equidistant from the origin. So, for meeting the condition for spherical design, the design points should be located at square root of k, where k is the number of factors, the value of alpha for k is equal to 3 is 1.682 for a rotatable design and it is 1.732 for a spherical design. Coming again in the above table, it can be seen that the value of alpha for k is = 3 is 1.682.

So, this is actually meant for a rotatable design but this value of 1.682 is not = 1.732, which is corresponding to square root of 3, here k is = 3 for a factorial design with 3 factors and hence this alpha value is 4th root of it, which is 1.682 and not square root of 3, which is 1.732, so all the design points in a rotatable design or not equidistant from the center and the design is not completely spherical.

So, if you look at central composite designs with k is = 2 and k is = 4, for k is = 2, it is 1.414 for a rotatable design and square root of 2 for a spherical design or a circular design, if you want to put it that way, so square root of 2 is = 4th root of 4, square root of 2 is = 4th root of 2 power 2, the number of factorial points, so both of them are = root 2, so the design is both spherical or mean, if you want to take it for a 2 dimensional case, circular and also rotatable.

But when you take k is = 3, you are getting 4th root of 8, which is 1.682, which is not = square root of k, which is 1.732, so even though the design; rotatable design is not strictly spherical, the values of 1.682 and 1.732 are pretty close to each other and so we are getting a nearly spherical design for k is = 3. Now, coming to k is = 4, we are having 16 factorial points and the 4th root of 16 is 2 and the square root of 4 is also = 2.

So, for this case, we have both the conditions of rotatability and a spherical design being met, so for both k is = 2 and k is = 4, the design is both spherical as well as rotatable, this design points are equidistant from the center and the design also is rotatable but when you look at a factorial design with 5 factors, the condition of both rotatability and sphericity is not met simultaneously.

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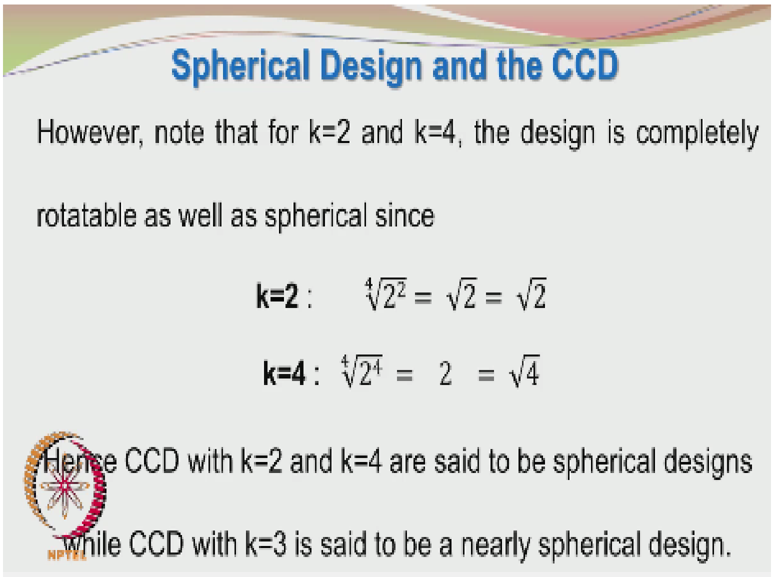

So, to reiterate what we say just now for k is = 2, we have for a rotatable design 4th root of 2 power 2, which is root 2 and that is = root k, the condition required for a spherical design. For k is = 4, the condition of rotatability stipulates 4th power of 2 power 4, which is 2, which is also = root of k is = 4 and hence we have both spherical as well as rotatable characteristics for the central composite design with either 2 factors or 4 factors.

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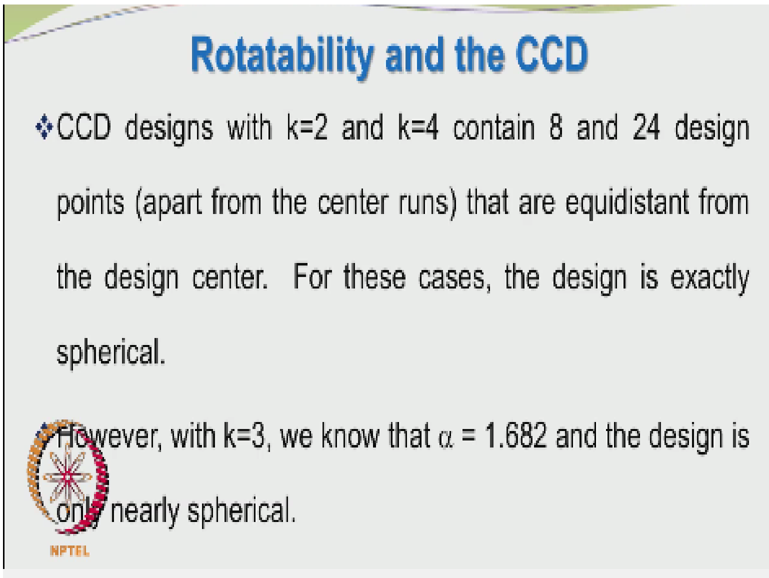

When you look at a central composite design with 3 factors, it is said to be a nearly spherical design because 1.682 and 1. 7321 are not very further apart. So, central composite designs with k is = 2 and k is = 4 containing 8 and 24 design points apart from the center runs that are equidistant from the design center. For these cases, the design is exactly spherical, however for k is = 3, the axial points are located at 1.682 and the design is said to be only nearly spherical.

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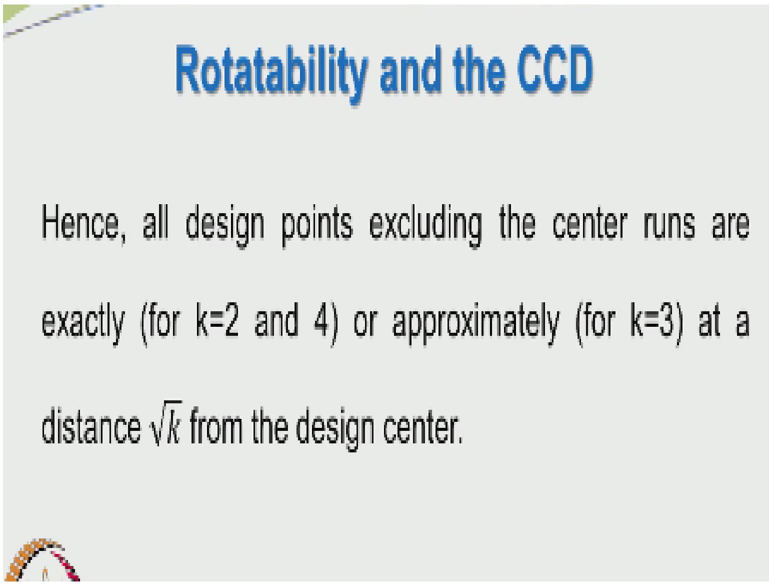

For k is = 2 and 4, the design points are exactly at root k from the design center, whereas they are only approximately so for a design involving 3 factors.

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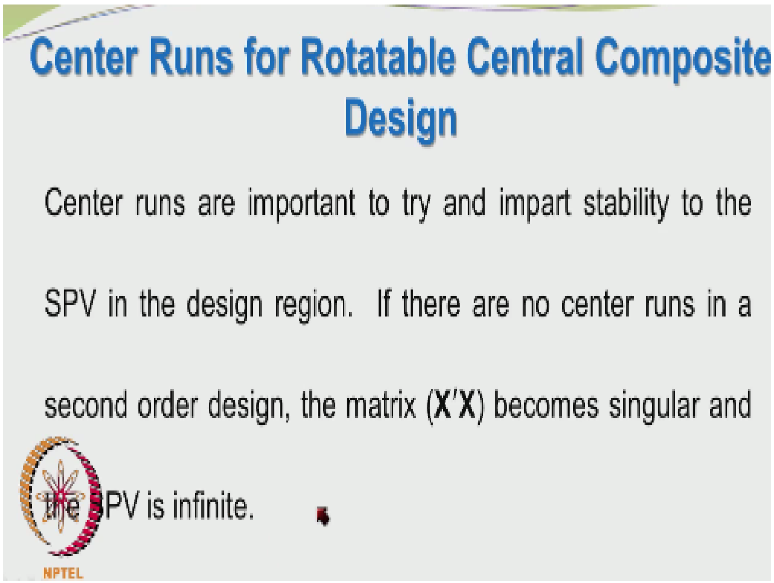

So, now we are looking at center runs, the importance of center runs we already emphasized as estimation for pure error to detect the curvature effects significance in the model. Now, we are going to see another role played by center runs in the central composite design. For a rotatable central composite design, it is actually rotatable central composite design, so center runs are important to try and impart stability to the scaled prediction variance in the design region.

We saw that not necessarily; the scaled prediction variance should be high only in the design boundaries or design extremes but it is also possible for the scaled prediction variance to shoot up in the center of the experimental design space. So, to have a check on that we increase the number of center points. If there are no center runs in a second order design, the matrix X prime X becomes singular and the scaled prediction variance is infinite.

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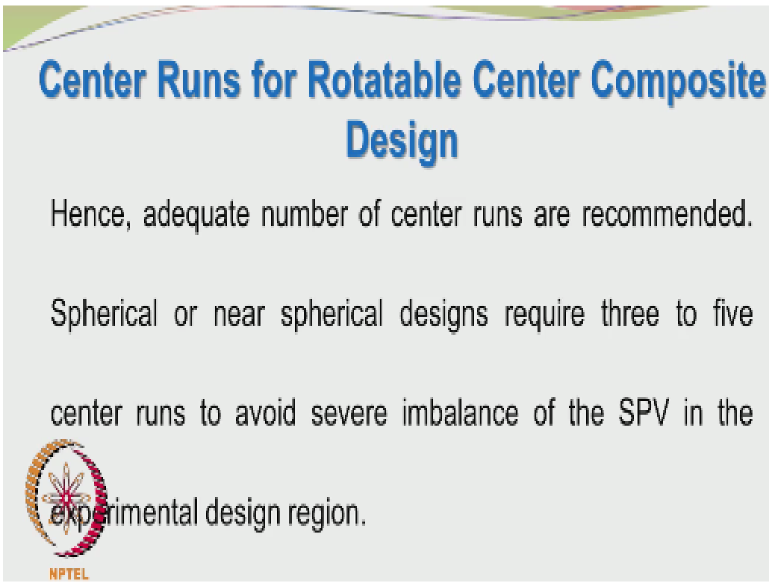

So, adequate number of center runs are recommended, spherical or near spherical designs require 3 to 5 center runs to avoid severe imbalance of the scaled prediction variance in the experimental design region. So, for factors ranging from 2 to 4, it is advisable to have 3 to 5 center points, so that the scaled prediction variance does not shoot up.

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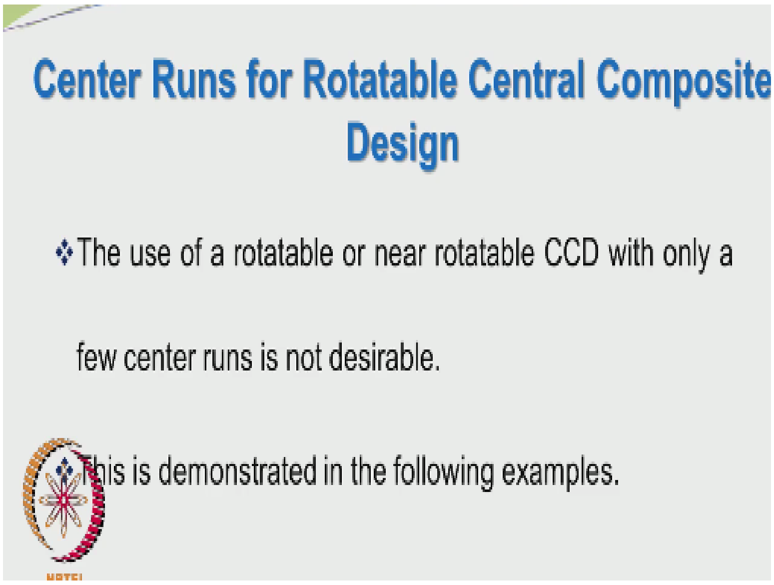

And when you are going in for a rotatable or a nearly rotatable central composite design, a few center runs only is not decidable, so adequate number of center runs are required for rotatable and nearly rotatable central composite designs. Recommended that you use at least, 3 to 5 center runs to avoid severe imbalance of this scaled prediction variance in the experimental design region.

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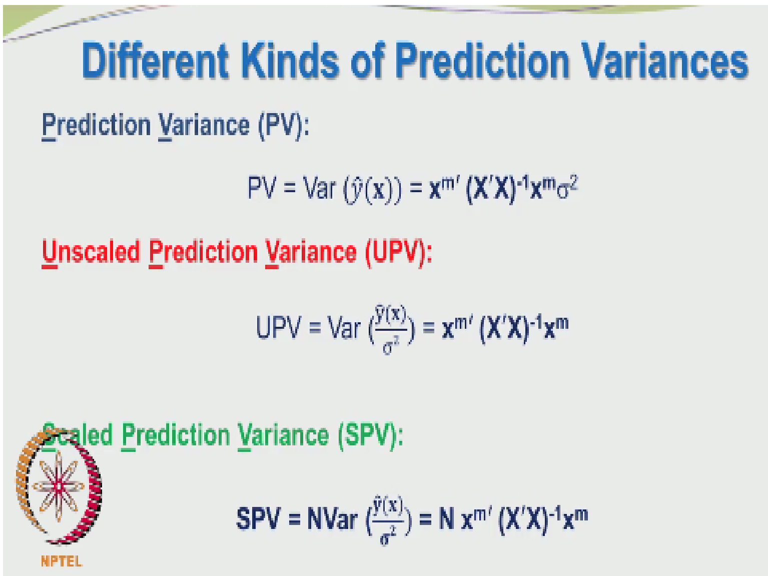

It is not desirable to have very less number of center runs for the rotatable or nearly rotatable CCD. So, we will demonstrate the importance of center runs with a few examples in the next lecture. So, thanks for your attention.