Course material

Course:

ENG606 / PHYS 442

Video:

DOE-Lesson14_part2-Mixture

Concepts (extracted from automatically generated subtitles):

Type of models. Simplex lattice design. Experimental point. Quadratic model. Quadratic terms. Sum of the factors. Real two-dimensional problem. M value. Situation of mixture. Constant linear terms. Cubic situation. More global discovery of your surface. Good cookies. Full cubic model. Shape of a quadratic model.

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(within ENG606 / PHYS 442.)

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notes

summary

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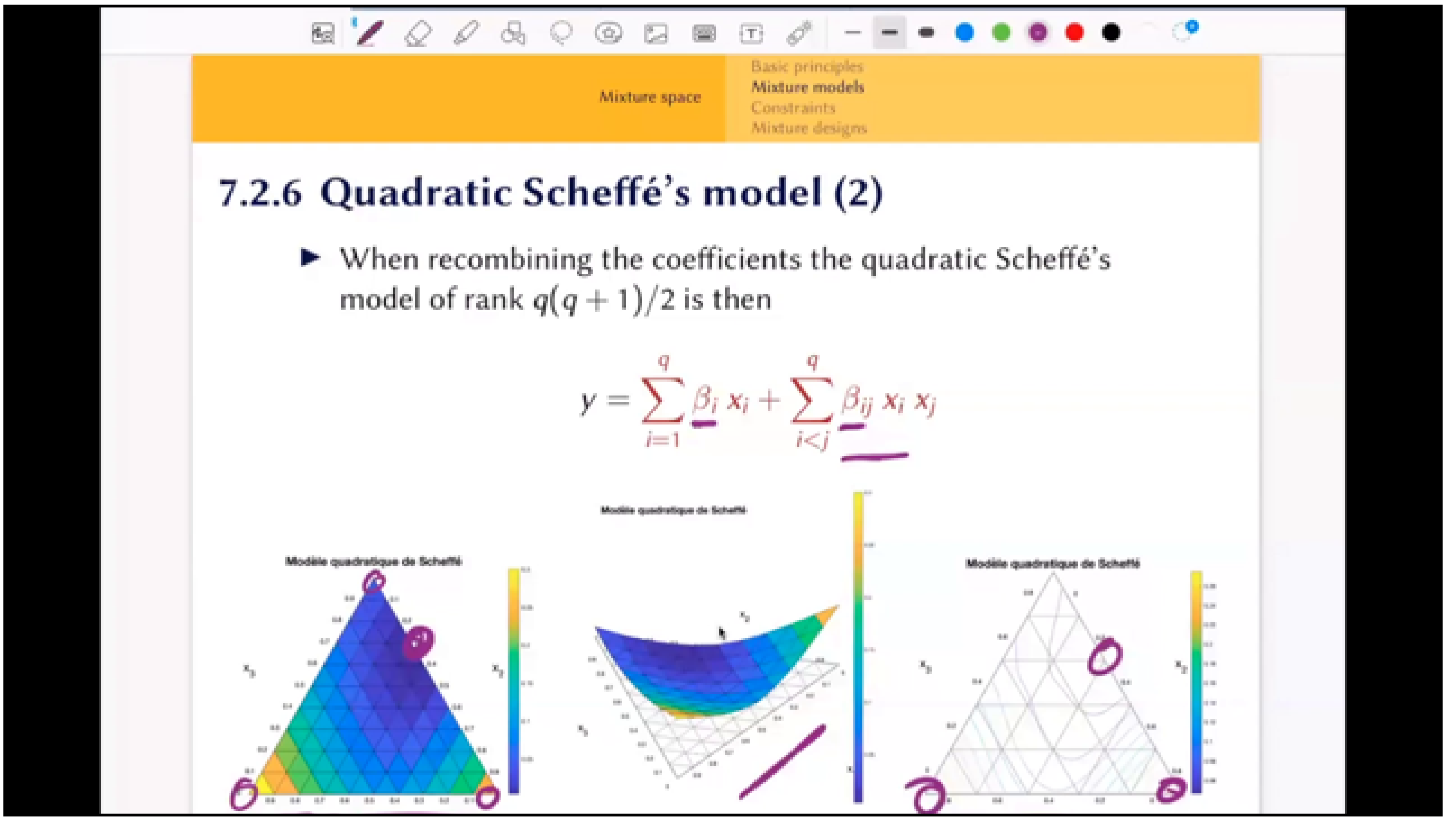
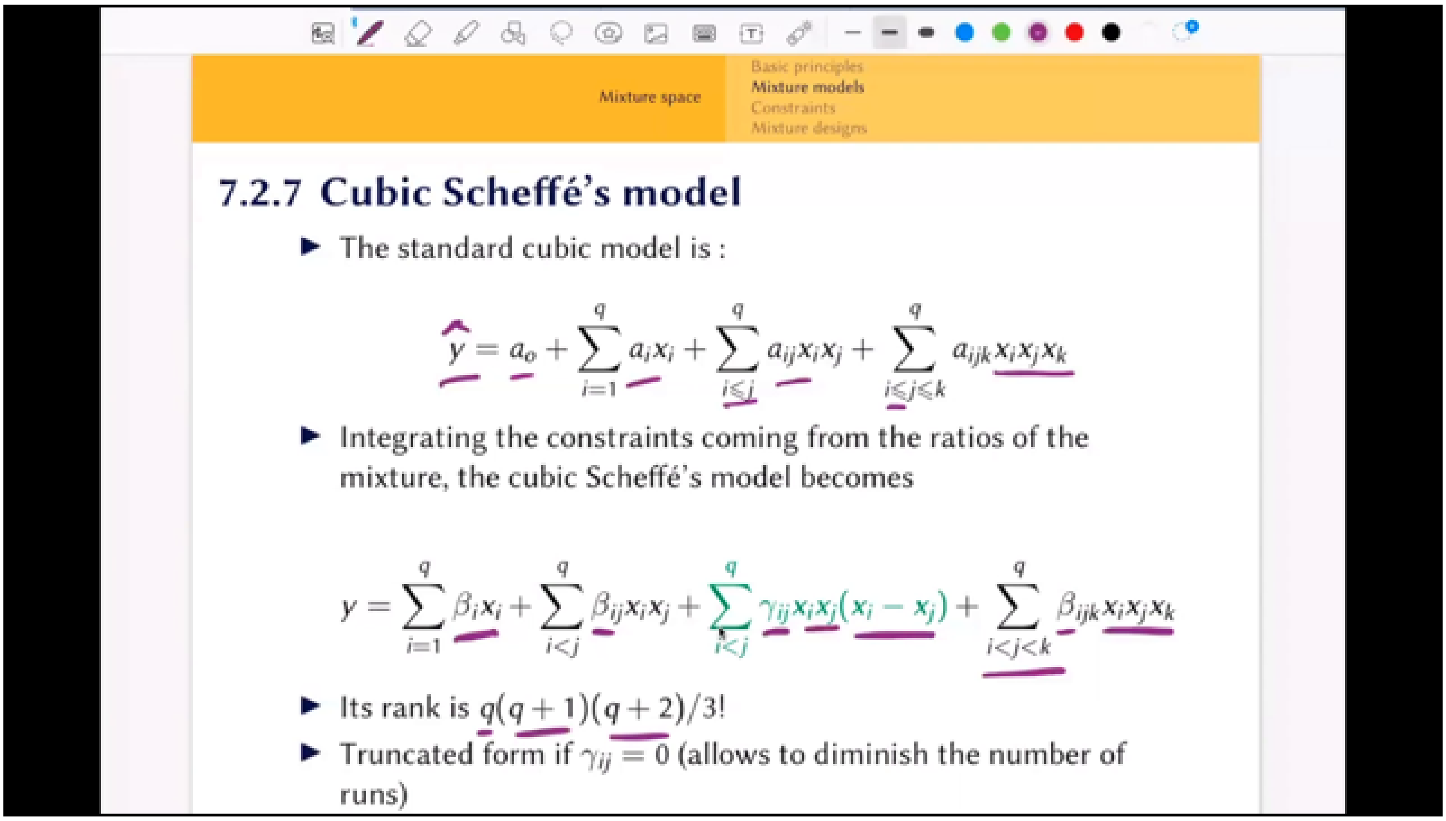


These subtitles have been generated automatically Okay, so let's continue this type of models.

notes

summary

0m 1s



So we have now see that we have a quadratic model without quadratic terms, but that is the shape of a quadratic model. We can also have a cubic situation. It seems that it's more common to go in cubic model with the situation of mixture than we do usually in standard situation. We continue with the same idea. So that means that we have a model which is a constant linear terms, quadratic terms, including pure quadratic terms and also cubic terms. And as we have I smaller or equal to j smaller or equal to k, we have the pure cubic term. So when we integrate the sum of the factors equal one, in this, we finish finally with the, all times the same way was linear terms, beta, with second degree terms, beta ij and two types of different third degree terms. We find a series of, we call them beta because it's as before. So all the possible but i smaller, strictly smaller than j, strictly smaller than k. So we do not have iij and iii and all this term. So all the indices here are different. One two three standard if we, we stress factor, we are within a ternary plot. And we have all the terms that have been called gamma for differentiating them from the previous one and especially differentiating them of the beta ij terms. You see they have two indices ij. So it exists by pairs. There are gammas as the same numbers and pairs of coordinates. So if we have three factors, that means that we have three possible gamma j, one two, one three and two three. And it's the product of two of the factors multiplying the difference of the two factors. The rank of the model now will be k, k plus one, k plus two divided by three factorial. And sir, let's say we have

notes

summary

0m 8s

7.2.7 Cubic Scheffé's model

- The standard cubic model is :

$$\hat{y} = a_o + \sum_{i=1}^{q} a_i x_i + \sum_{i \leqslant j}^{q} a_{ij} x_i x_j + \sum_{i \leqslant j \leqslant k}^{q} a_{ijk} x_i x_j x_k$$

- Integrating the constraints coming from the ratios of the mixture, the cubic Scheffé's model becomes

$$y = \sum_{i=1}^{q} \beta_i x_i + \sum_{i<j}^{q} \beta_{ij} x_i x_j + \sum_{i<j}^{q} \gamma_{ij} x_i x_j (x_i - x_j) + \sum_{i<j<k}^{q} \beta_{ijk} x_i x_j x_k$$

- Its rank is $q(q+1)(q+2)/3!$
- Truncated form if $\gamma_{ij} = 0$ (allows to diminish the number of runs)

two, two possibilities. We can have a truncated cubic model or full cubic model.

notes

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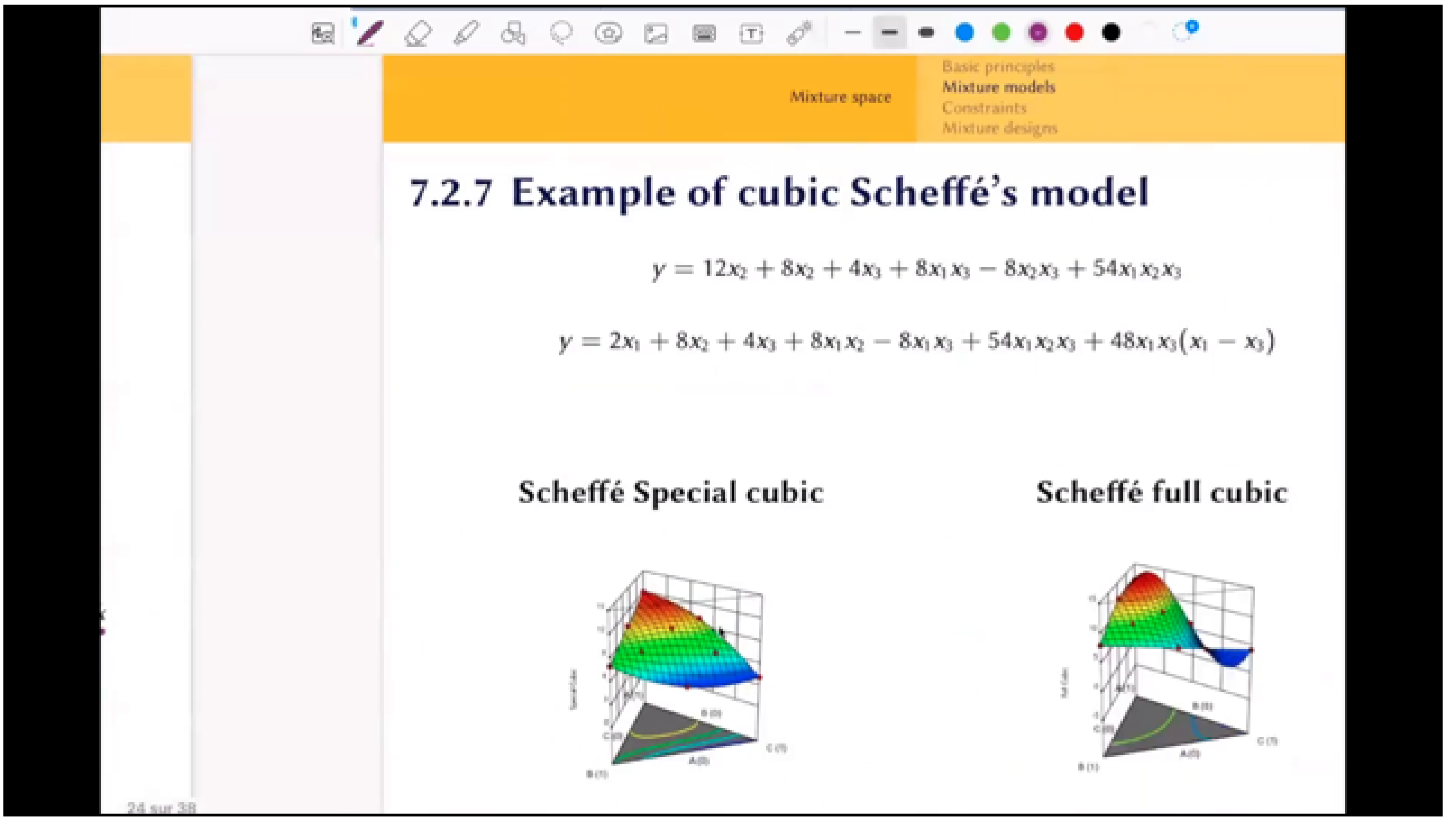
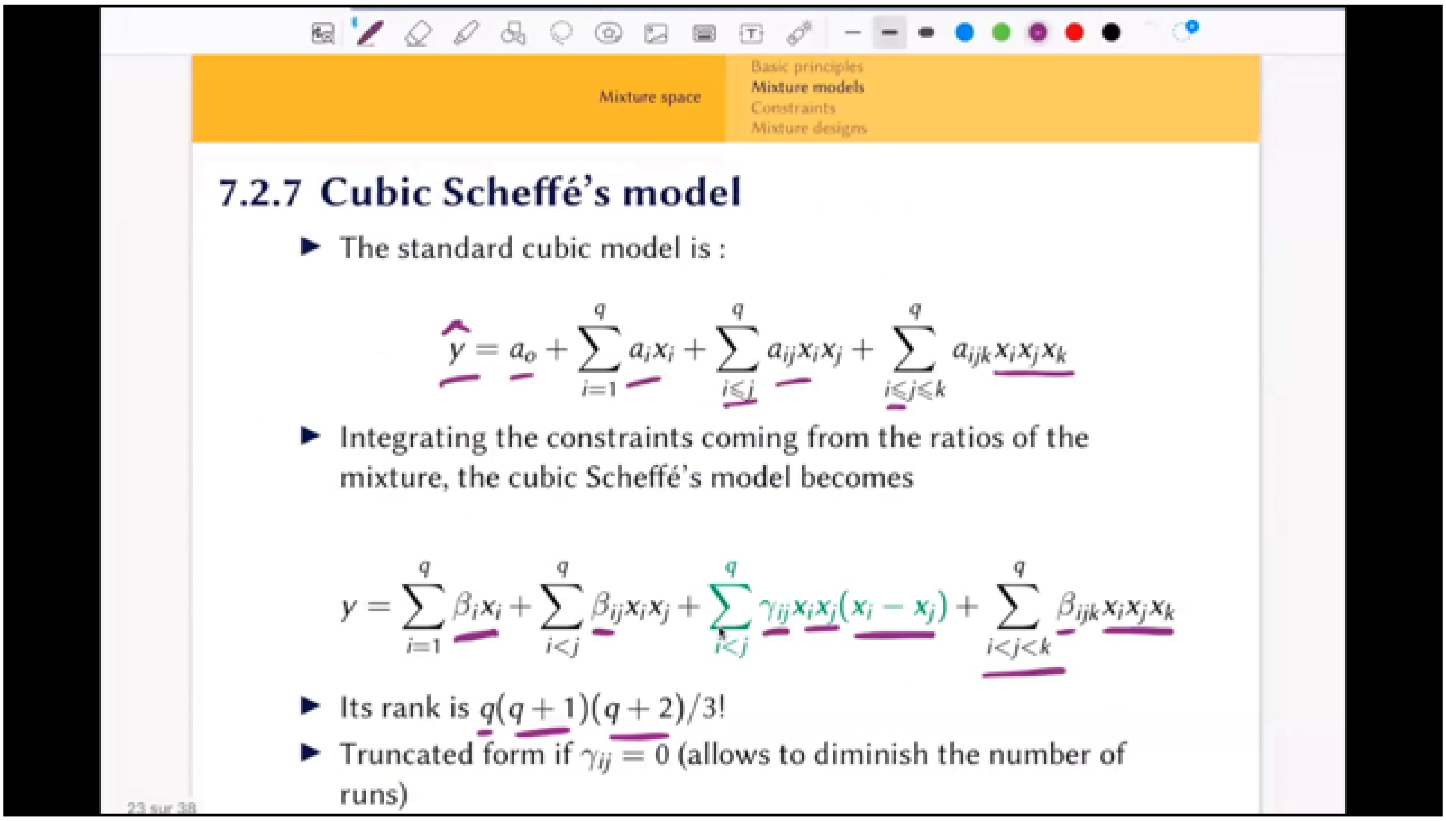


In the next slide, I show you what could be the difference

notes

summary

3m 25s

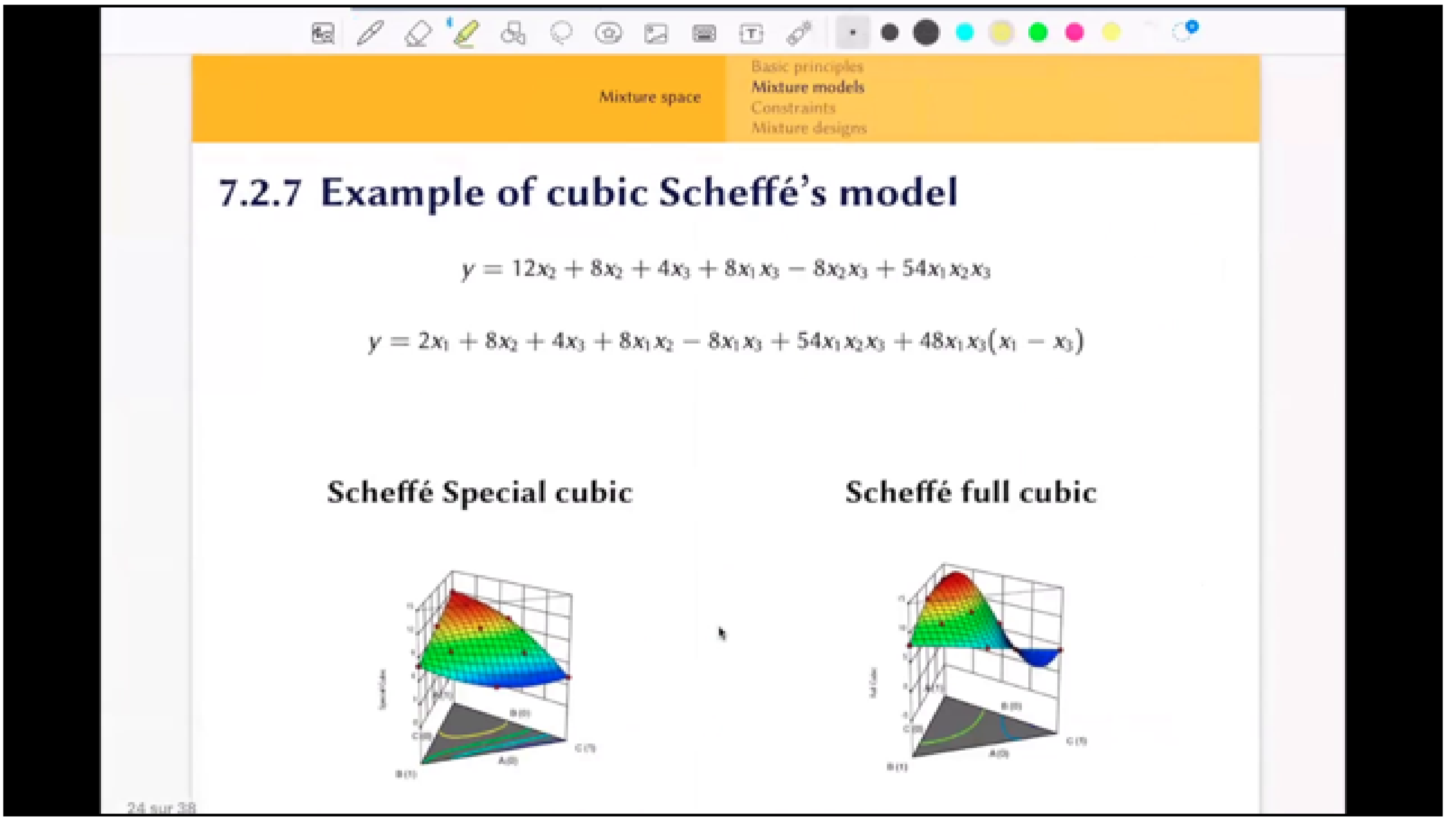


after it's a decision if you have sufficient movement, sufficient degree of freedom in your measurement for the chef's fulls cubic. Eventually you use the fulls cubic if the the special terms are significant or if you are not, you have the possibility to have just the truncated cubic model. So sometimes people don't say truncated cubic model because just chef and it's typical of the

notes

summary

3m 27s

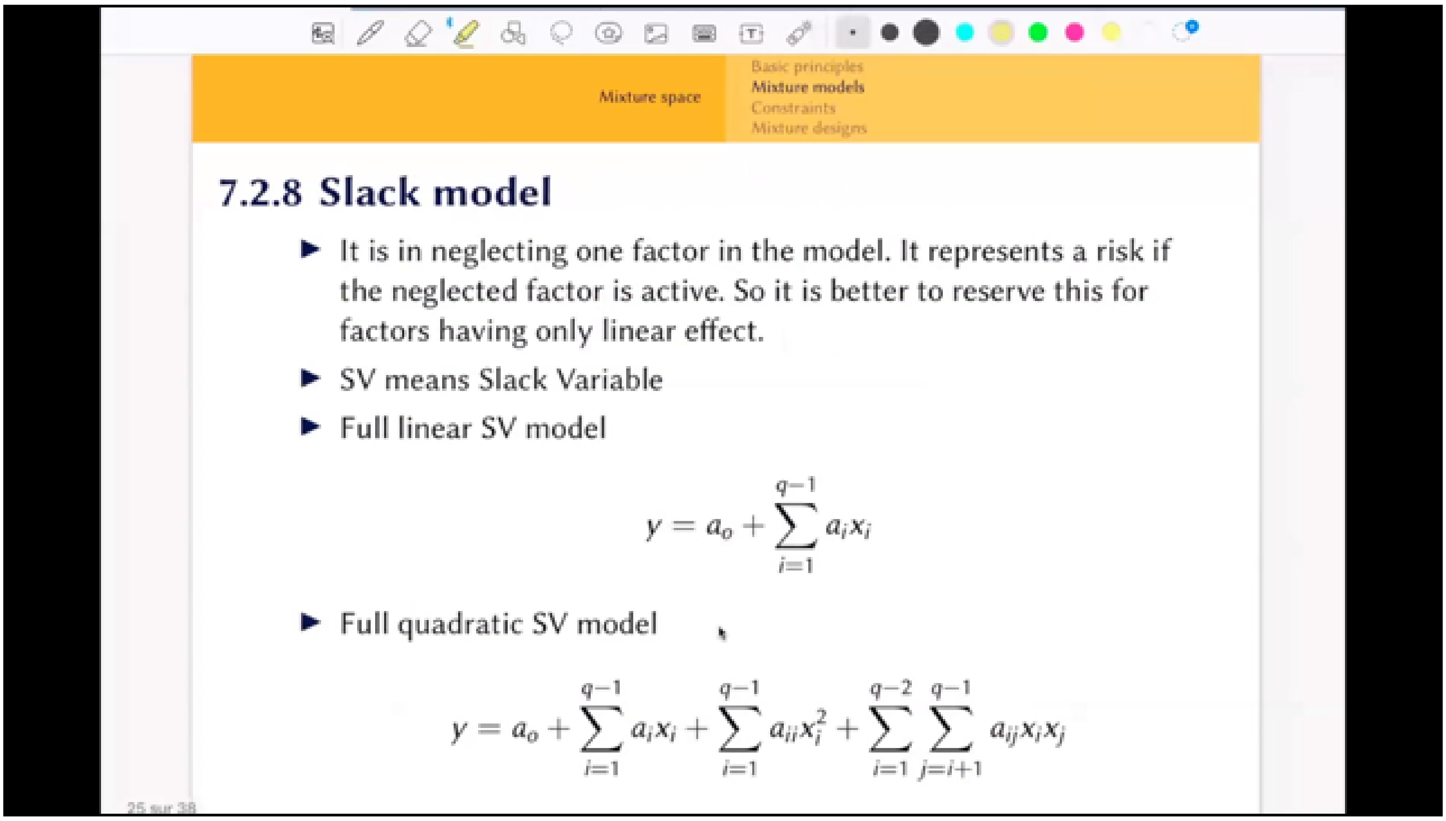


chef model. You have to change of color for what I'm saying. So you have the beta. So if you have only the beta, usually it's called a cubic chef model. It is a truncated model that we call it cubic model.

notes

summary

4m 5s

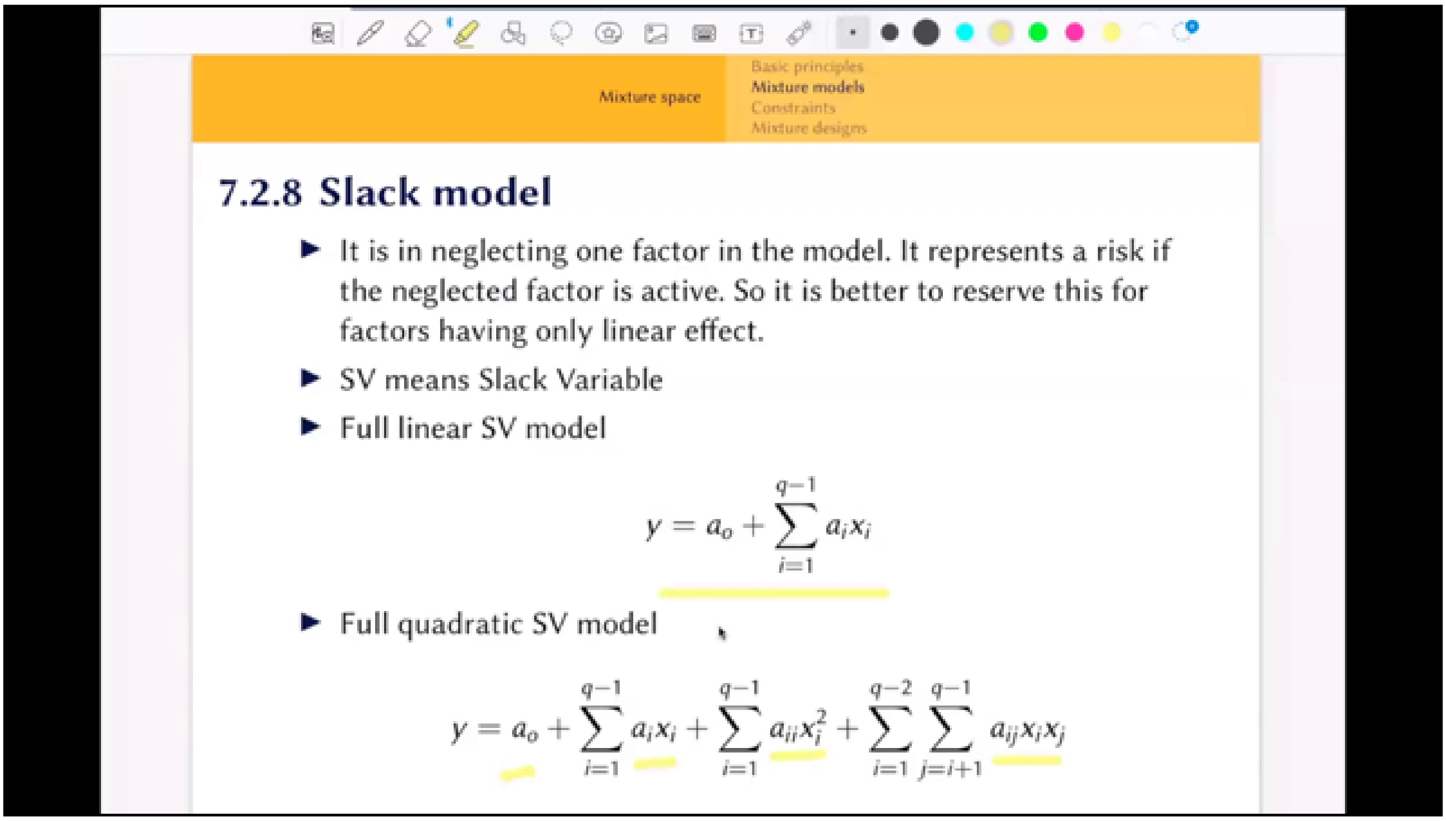


And so when you have the gamma, it's called the full cubic. So it's make a small detail in the surface. After it again, it could be depend if you are rich, you can make sufficient experiment for having sufficient degrees of freedom in your data and you can do this. Sometimes you are more interested in a more global discovery of your surface and eventually you just do a special cubic model. You have two examples and you go to what's what's look like. Okay, so this was for trying to illustrate it was a chef model. Usually you can do most of the thing with the quadratic and the linear model, but eventually the cubic model. I even see some time in some papers going to more degrees, but I will not include that in my course.

notes

summary

4m 26s

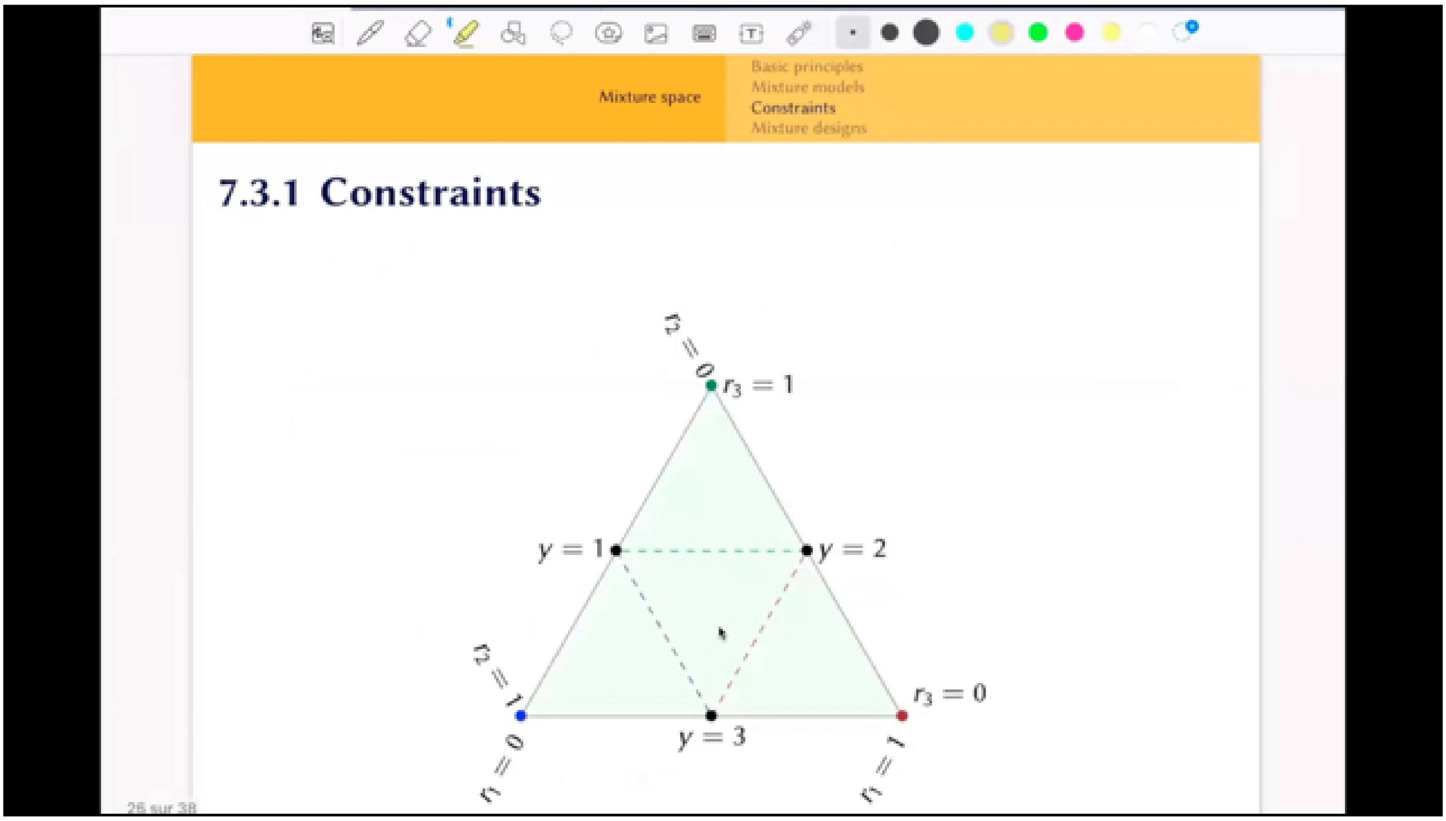


In the slack model, not a lot of things to say except that you have a constant. So a full quadratic will have a constant sum of linear terms with one missing because with the slack model, so we have n minus one linear terms and is the same thing for the pure quadratic terms where we have q minus one. So q was the numbers of factors. It was also the rank sometimes in this theory they call that rank. And for the instruction terms, you also are not. So in your model, you will have one factor which is disappearing. Again, it worked very well. You can do that. The only thing that you can have a factor that could be quite very important and it never appear in your situation. So it's very evident you are making the recipe for making good cookies and you never have sugar. Okay. People say, oh, it's a recipe without sugar, but in fact, sugar. Here is the last factor. Is the slack model. In fact, you can hide some product by you hide.

notes

summary

5m 29s

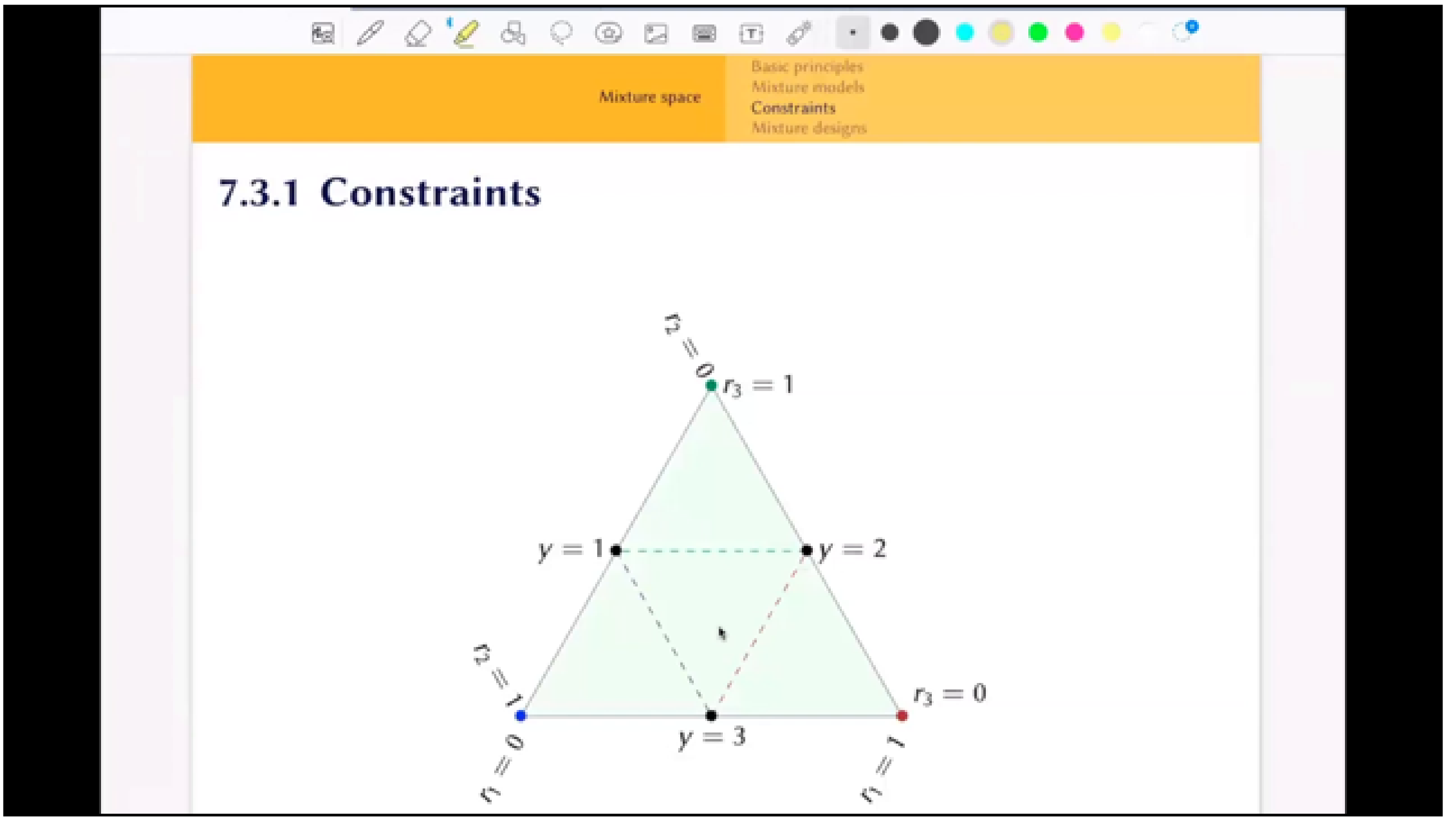


You don't hide it, but I say it doesn't appear. And this could be the only tricky aspect of it. Okay. So this is with my model. Sheffa's model, slack model, Sheffa's model are a little bit more sophisticated to Manat, but in fact, they have the advantage of presenting all the factors.

notes

summary

6m 49s

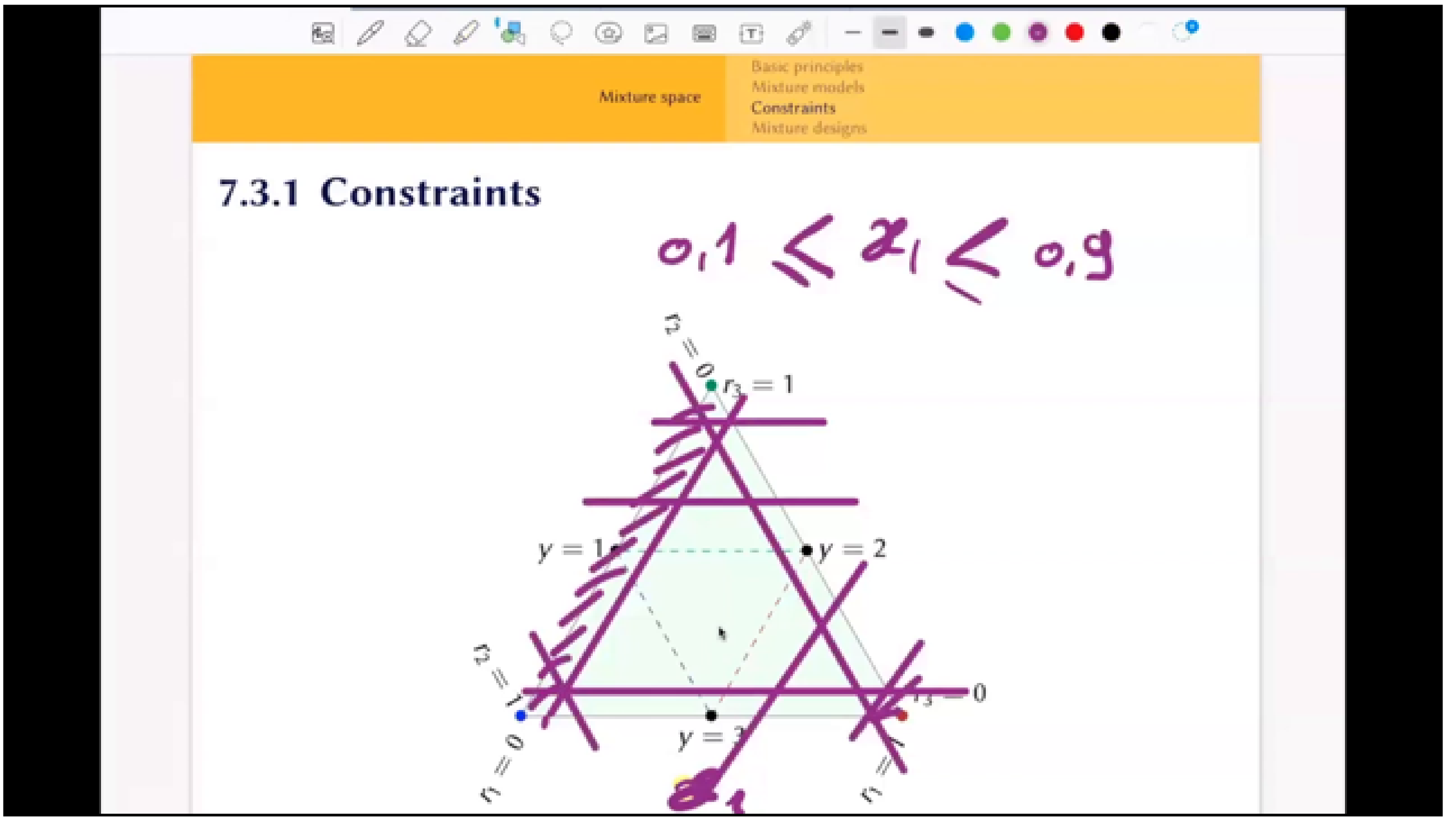


After it's out, we represent the constraint in this thing. So the constraint are most of the time linear constraints. So we say that one of the factors should not be higher or smaller than a given value.

notes

summary

7m 7s



Imagine that the constraint is in the X1, which is here. So if we say that we want to have X1, which is between 10% and 90%, can you imagine how this will have as a consequence? That means that we have to detect X1. Imagine that the 10% is here. Imagine that the 90% is here. And we have the is all line for the line corresponding of the same value of X that are those lines and those lines. So that means that now my space is what stay in green. So if we have the same type of constraint in all the factors, it's okay. Finally, we will finish with so it will depend the size of the, but it will perhaps finish with something like that and something like that. Finally, we can finish with a space if it's the constraint are equal in each of the factors, we will finish with a triangle in this situation. If it's not the case, well, we can finish with something more complicated depending on the type of limitations that we have. Again, if the limitation are the same in all the axes, it's very easy. It will be a triangle. If not, you have to look at it. And again, in one dimension, very easy. In two dimensions, three dimensions is also not so complicated. In three dimensions, in the tetragons, if you have to have planes of limiting some surface, it became quite complicated. And afterwards, we will look at the designs. And the design will be, if you are still in a triangle experimental space, you will use the design I will present to you. If you are not in a triangle space, finally, eventually, you will come back to the second degree design I have present to you. You will try to draw an hexagonal space, or you will try to use a composite design

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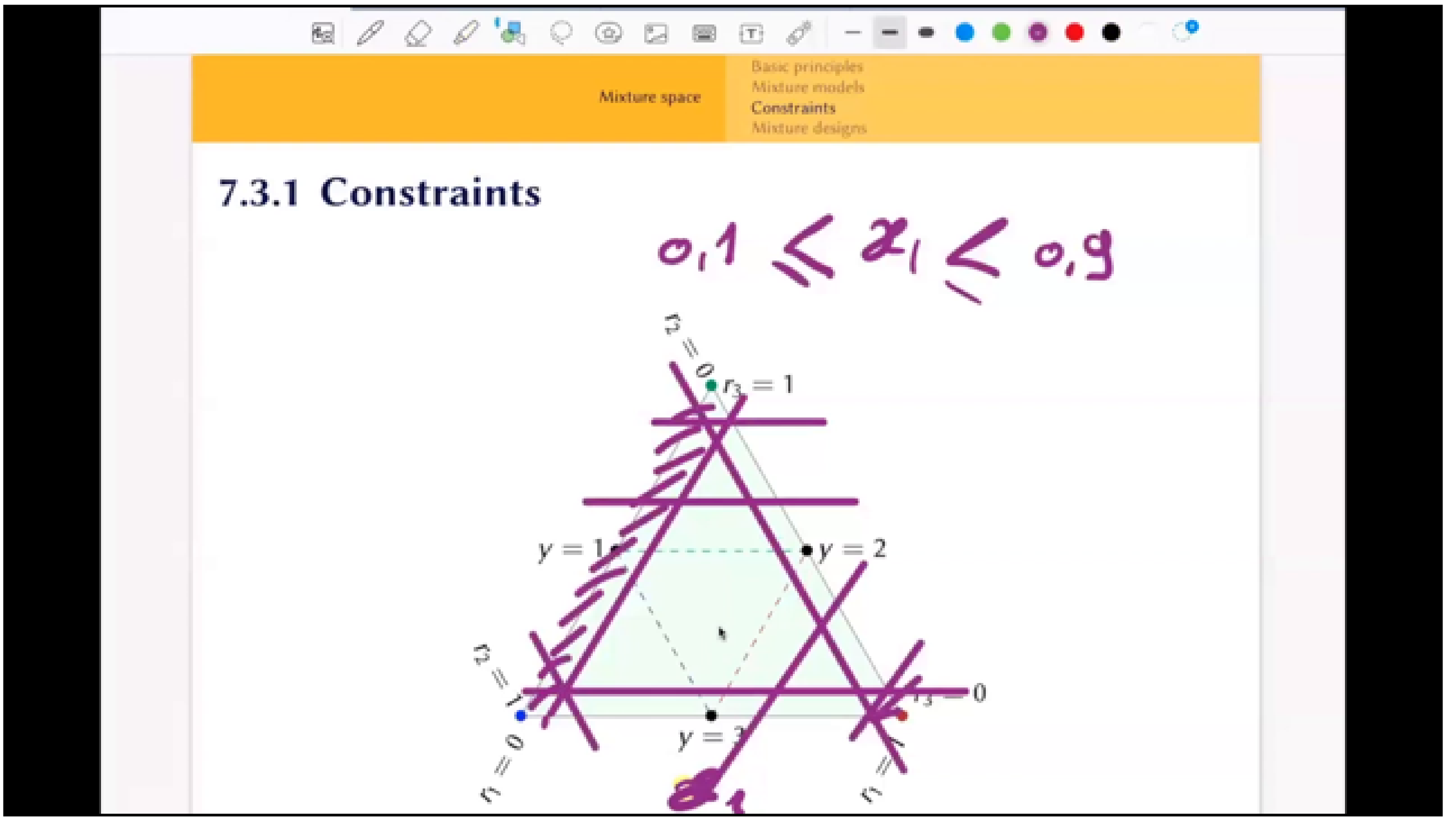
summary

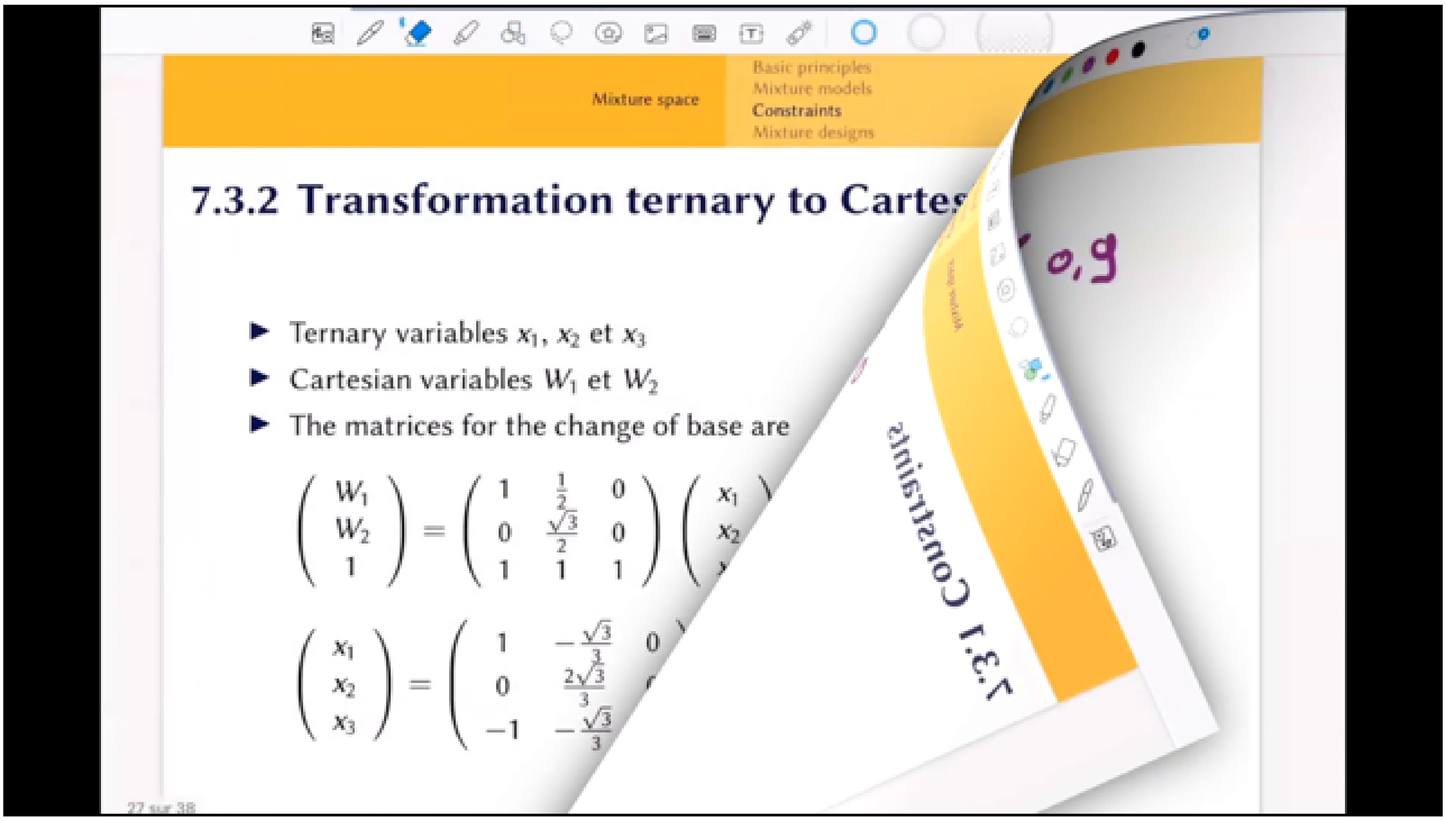
7m 29s



within this space for trying to have the better definition of the surface, but will be outside of the situation in which I will present you a few designs that are very good for triangular space. You are not anymore in triangular space.

notes

summary



So you really have to consider this limitation.

notes

summary

10m 13s

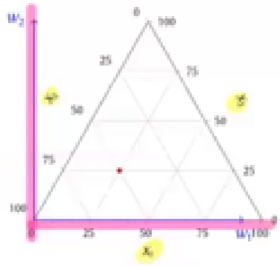
Mixture space | Basic principles | Mixture models | Constraints | Mixture designs

7.3.2 Transformation ternary to Cartesian

- Ternary variables x_1, x_2 et x_3
- Cartesian variables W_1 et W_2
- The matrices for the change of base are

$$\begin{pmatrix} W_1 \\ W_2 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 & \frac{1}{2} & 0 \\ 0 & \frac{\sqrt{3}}{2} & 0 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 & -\frac{\sqrt{3}}{3} & 0 \\ 0 & \frac{2\sqrt{3}}{3} & 0 \\ -1 & -\frac{\sqrt{3}}{3} & 1 \end{pmatrix} \begin{pmatrix} W_1 \\ W_2 \\ 1 \end{pmatrix}$$

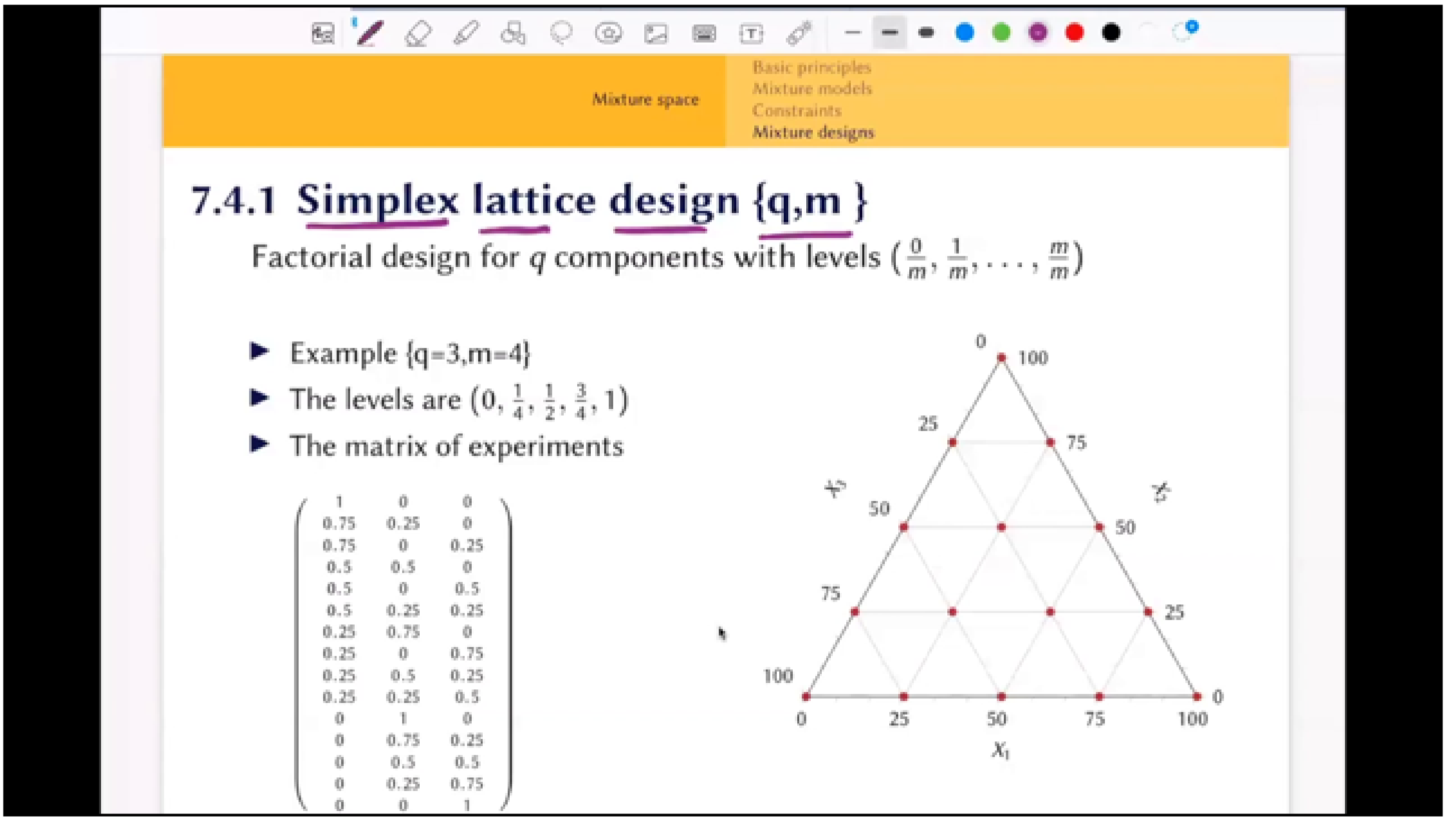


So sometimes when the surface is not anymore triangular, we could better think to a real two-dimensional problem. So you need to make a transformation of your variable. So you will have your problem variable. Let's call it x1, x2, x3. I will have my geometrical variable, I mean two-dimension, and I will call them y1 and y2. So you see here, I would have x1, x2, x3, but I can represent my problem with two variables, y1 and y2. This could be interesting. Again, if your surface, your final experimental surface is not a triangle, you would like to use de l'air design, composite design. You better think for making your design, you better think in two dimensions and in three dimensions with a shape which is not a triangle. So you need a transformation. So in this slide, you have the two transformations for going from a situation with three factors to a situation with only two directions. So one is not necessary, but I just wanted to have matrices that I can inverse or I have invent. I have an answer which was already fixed. I have fixed the one in my answer because I have one line of my of my matrix which is just make of one, so just change nothing.

notes

summary

10m 18s

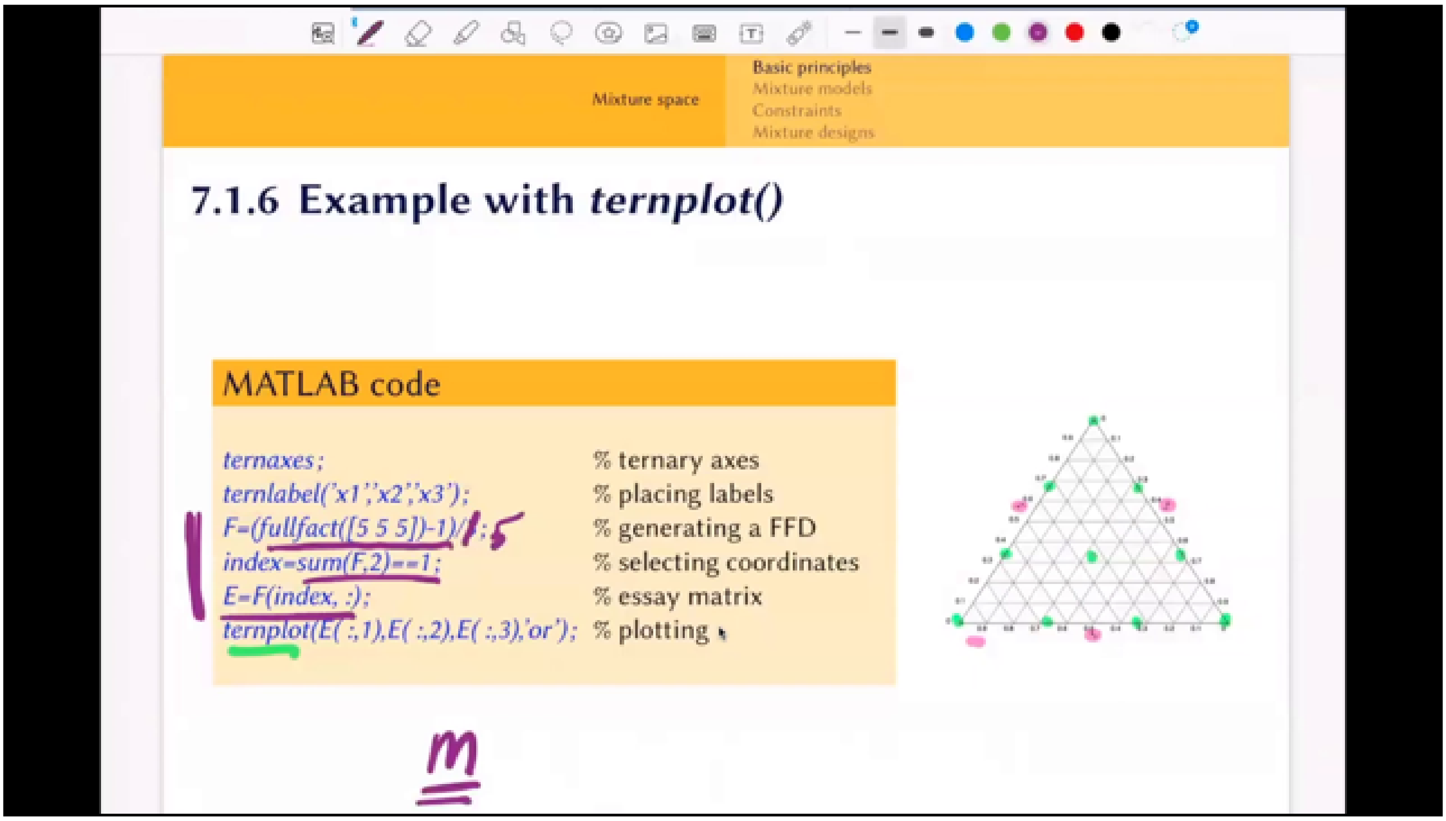


But it gives me the advantage that I can reverse this matrix if I want and I can get the reverse system easily for going to a situation where I have two inputs and I finish with three outputs. Normally, I should have a matrix of two by three, but this type of matrix I cannot inverse it. So for me, it was easier to make things like that. So now I present you a few elements, a few tools around this. I can present you the standard design related to this type of situation. If your experimental space is a triangle, part of that it could work also with two real variables that represent a triangle space, it's a geometric. So something we called simplex lattice design. Simplex because you remember, I say that the word simplex is representing what happened when I am able to fill all the space. So it's simplex because I'm putting space all over my space. Lattice because I'm making a network, a lattice with my experimental point and it's a design.

notes

summary

12m 5s

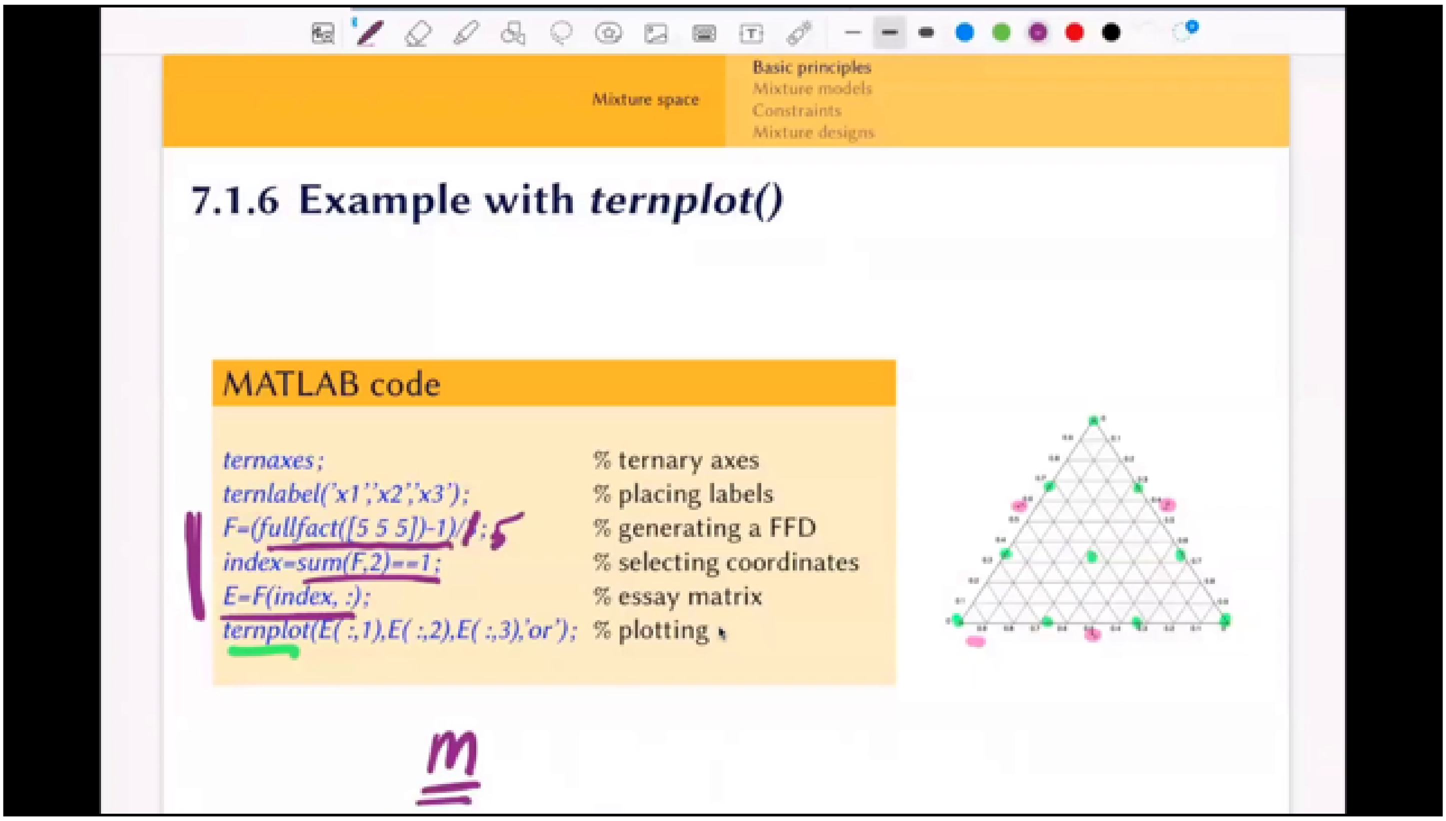


And so after q and m, q represents the number of factors and m is a number of levels that I want to use within my range for each of the factors. So m could be two. So if m could be two, I will have my segment for any of factors that will be divided in two. So I will have three points. I will have zero, one half and one. If m is three, that means that I will have three additional points, more zero. I will divide my things. So I will have zero, one, two and three. I will divide my segment in four. And so for having all those points, so here an example, if I have q equal three, I can work in the ternary graph. I have m, which is four. So that means that my level are zero divided by four, one divided by four, till four divided by four. So it makes me the different points, zero, one quarter, one half, three quarter, one. And then I will have my matrix of experiments that will be made by all the possibility, if it's sort of factorial situation, a full factorial situation, of all the possibility. But I need to have the sum of all my coefficients in one line, that must be one. So I can play to the n minus one element and the last one must be fixed. And like that, I have this simplex lattice design. And for that, I have to tell you that I make an error in my slides last week. So the slide, so seven, one, one, six, you have to correct. I have to divide by, I wanted to have six value in each axis. So I have m was equal to five, and I have to divide by one fifths and not one third. So if I have two birds, so this

notes

summary

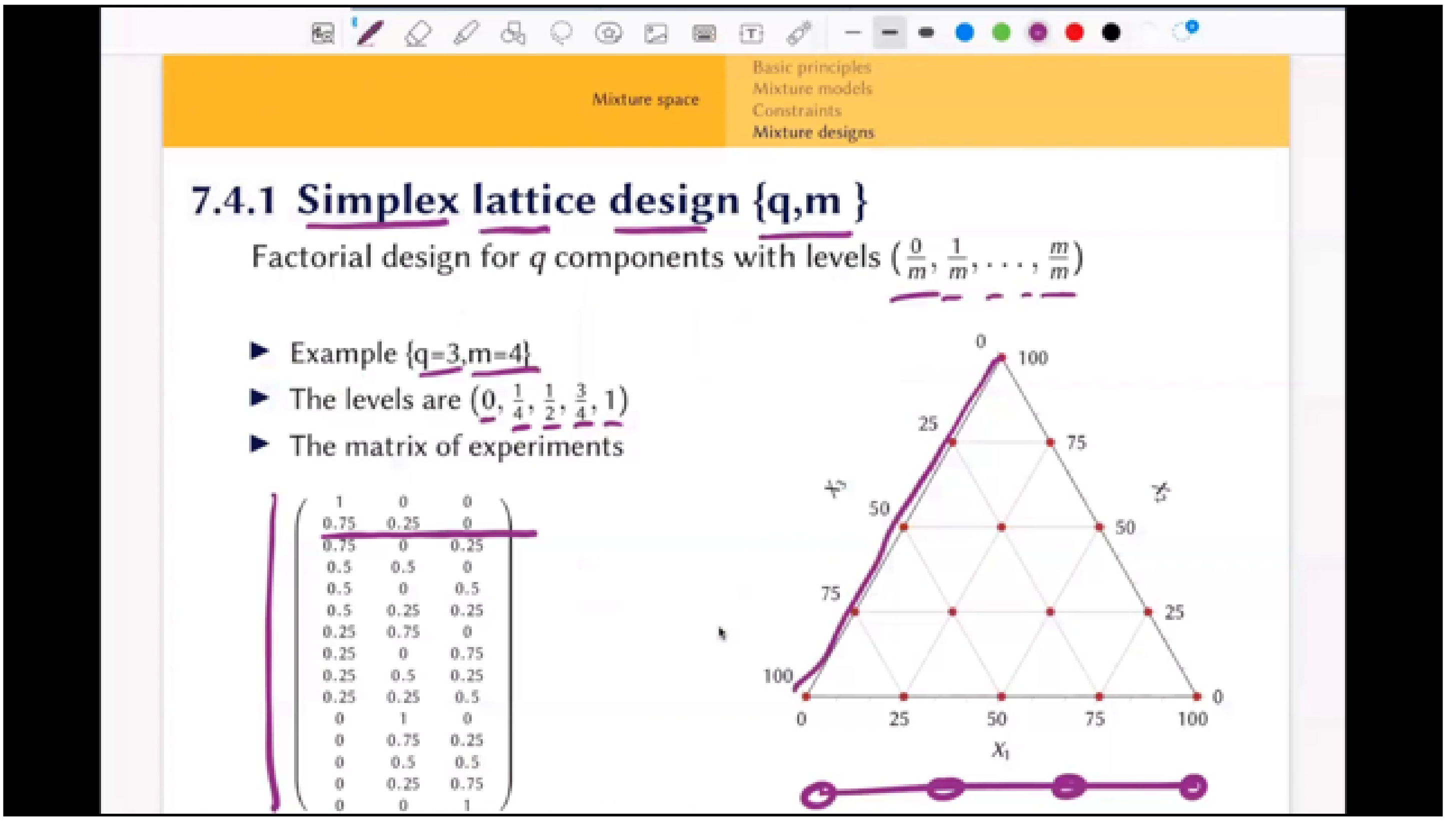
13m 37s



algorithm work also, this is a good algorithm for building this type of design. What I do? Okay, I decide the m, the m value. When I have decided m, I can build a full factorial matrix with all the possibility of having the different ratios of one, this case of one fifths in the other slide of one fourth. But not all the possibility will fit in my triangle. And so after I just choose the cases where the sum of the component is equal to one, and then I have my simplex network.

notes

summary

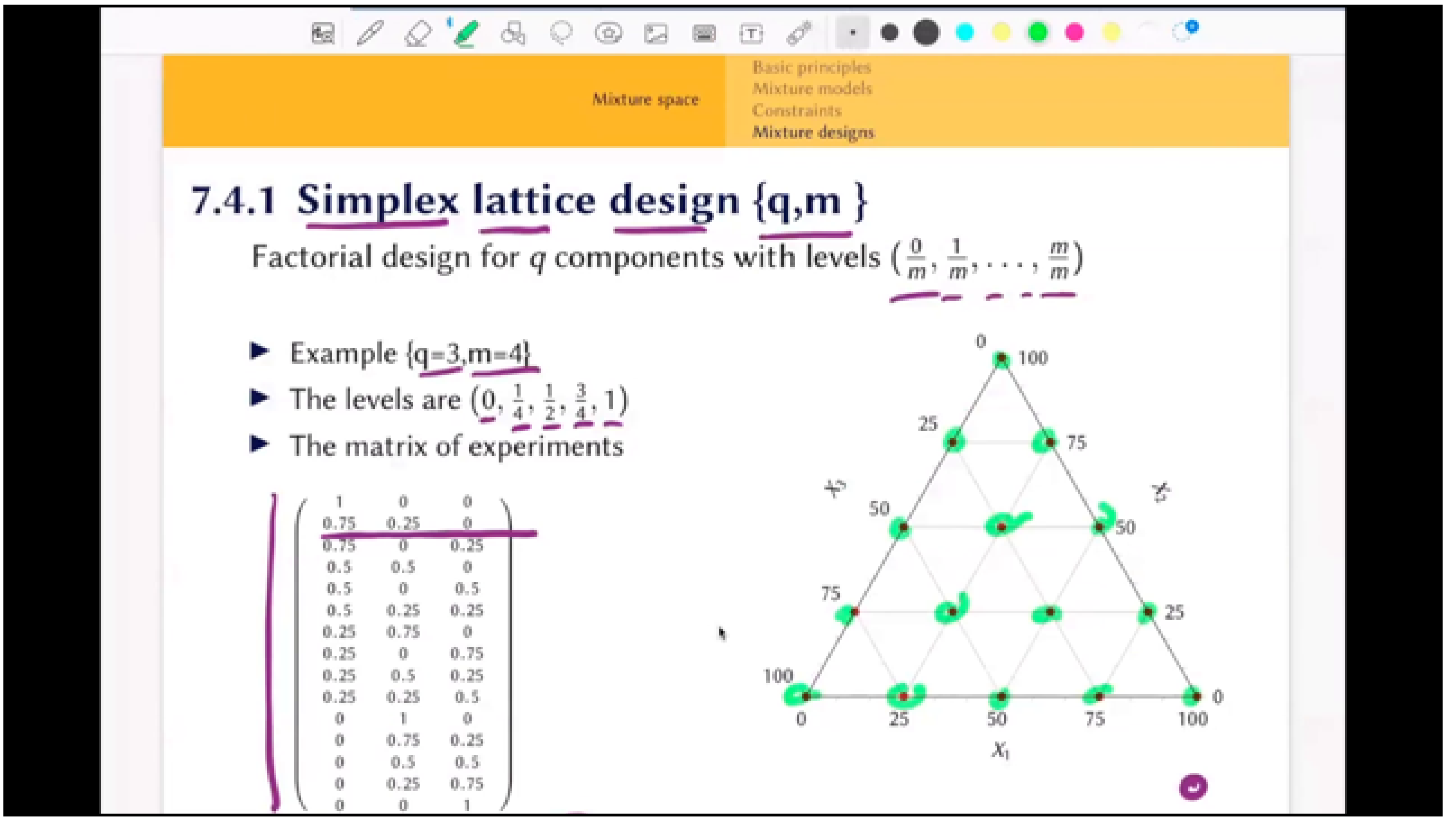


So the algorithm in 7.6 is explaining how you can build rapidly this matrix.

notes

summary

17m 1s

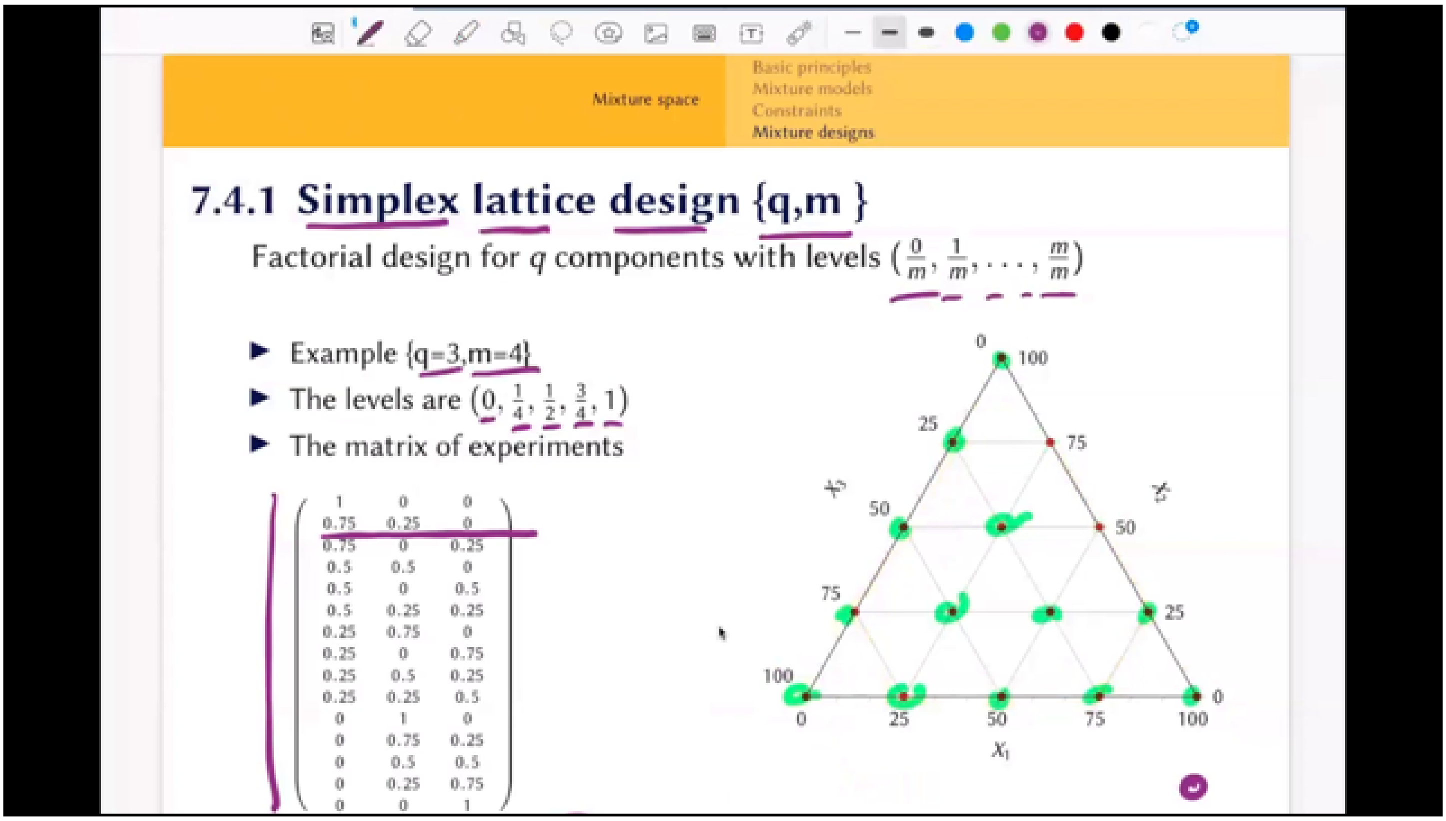


And so you can see in the ternary diagram what are the points that we get with this method. So we get all those points.

notes

summary

17m 7s

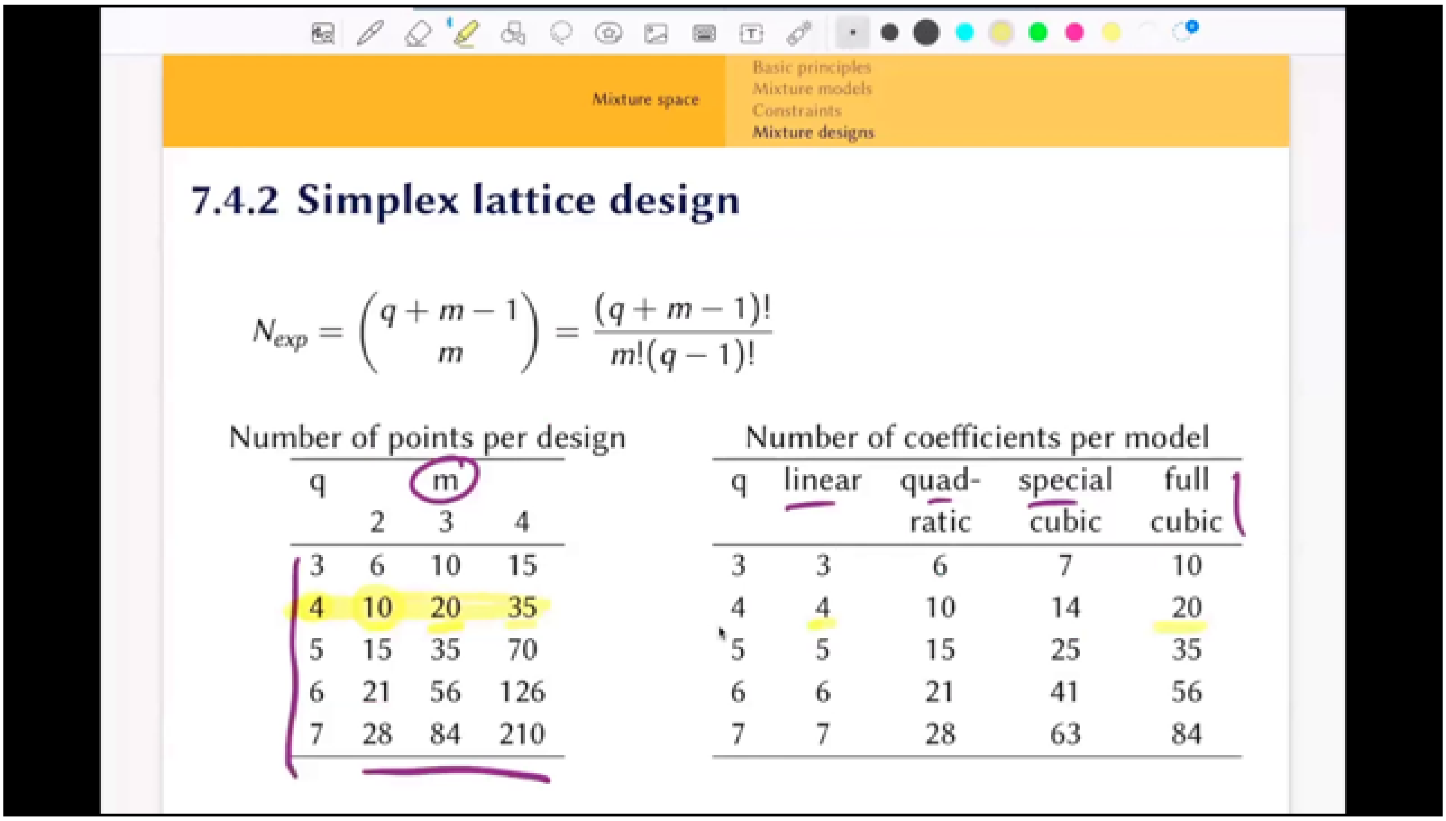


So what do you think could be the problem of this design? Problem of this design that most of the points, 7.6 is explaining, or you can, in this case, there are nine of the points are only two component products. Three are one component product. This are one component product. And only three are real full mixture. So this is real the problem of this design. So two solution, one will be the next slide.

notes

summary

17m 22s

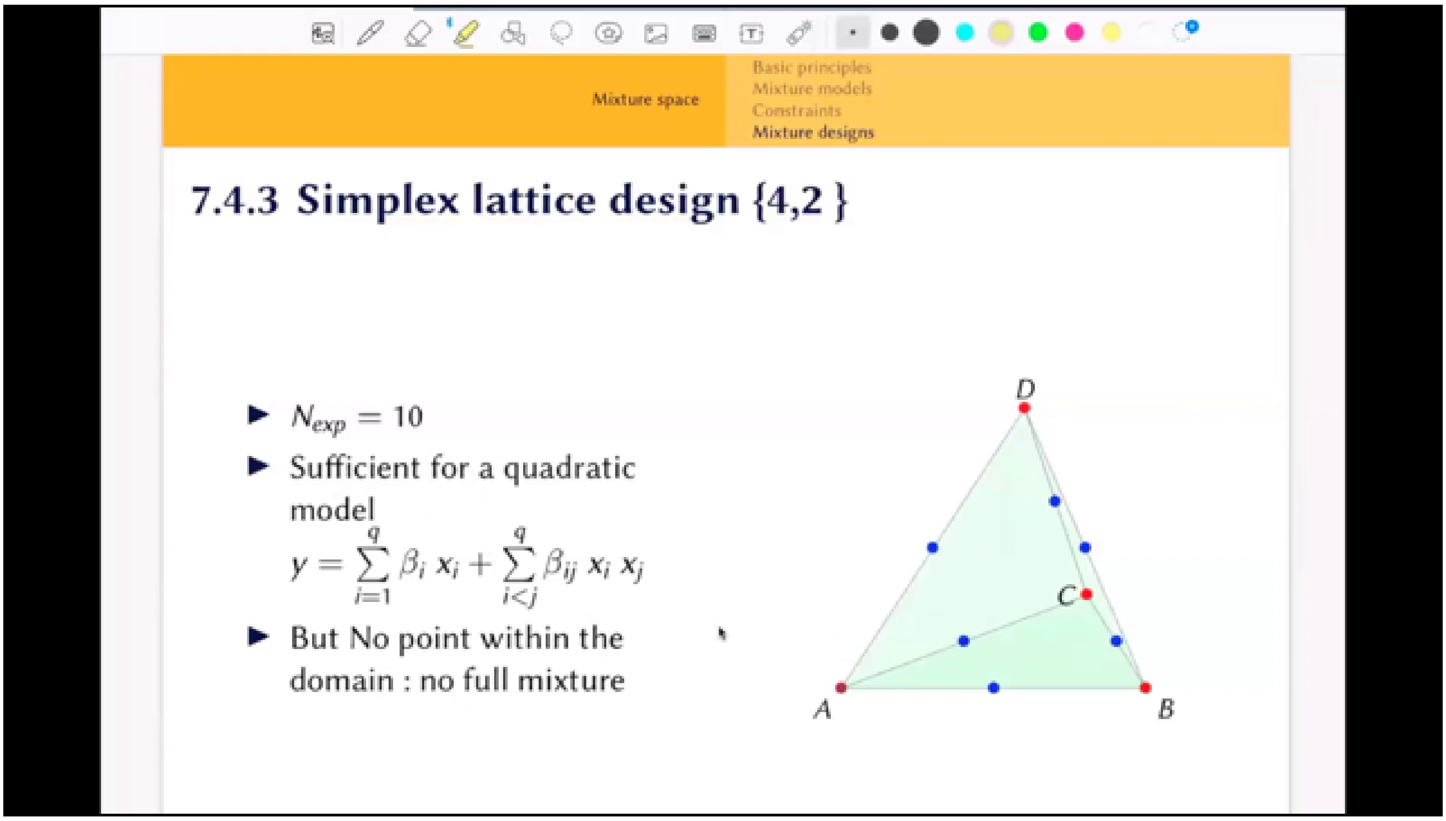


But you can also do something. You can say, okay, I will change my axis and having here, you can make limitation and say, okay, I don't want any product smaller than 10%, 1%. I don't know you decide what is what is reasonable as a space. So it corresponds to limited the triangle. So diminishing the size of the triangle, because if you say that each of one is higher than 10%, that means also each of one is also smaller than 90%. So it's like, it's the same thing as changing this axis and saying that this axis go to 10% to 90%. 7.6 is explaining, or you can for all the axis. And this is also a solution to avoiding this problem with this slide. Here, a few calculation with the slides with how many degrees of freedom you have, how many points, depending on the numbers of levels that you choose, how many levels. And you see also a front. I don't spend too much time on that. But it's also for the different model, which you need for having the good surface. Corresponding to the linear quadratic and special cubic or full cubic. So you see that if you have a situation with four products, so we are in a pyramid in a tetragon. If you use the simplex lattice, you can have 10, 20 of 35 points. And you see that so for a linear model, it could be okay to work with just m equal 2. I don't know if it's suitable for the problem of having a pure mixture or having all component mixture. And with m equal 3, you have sufficient data points for making full cubic models. So those designs are okay. They are powerful.

notes

summary

18m 4s

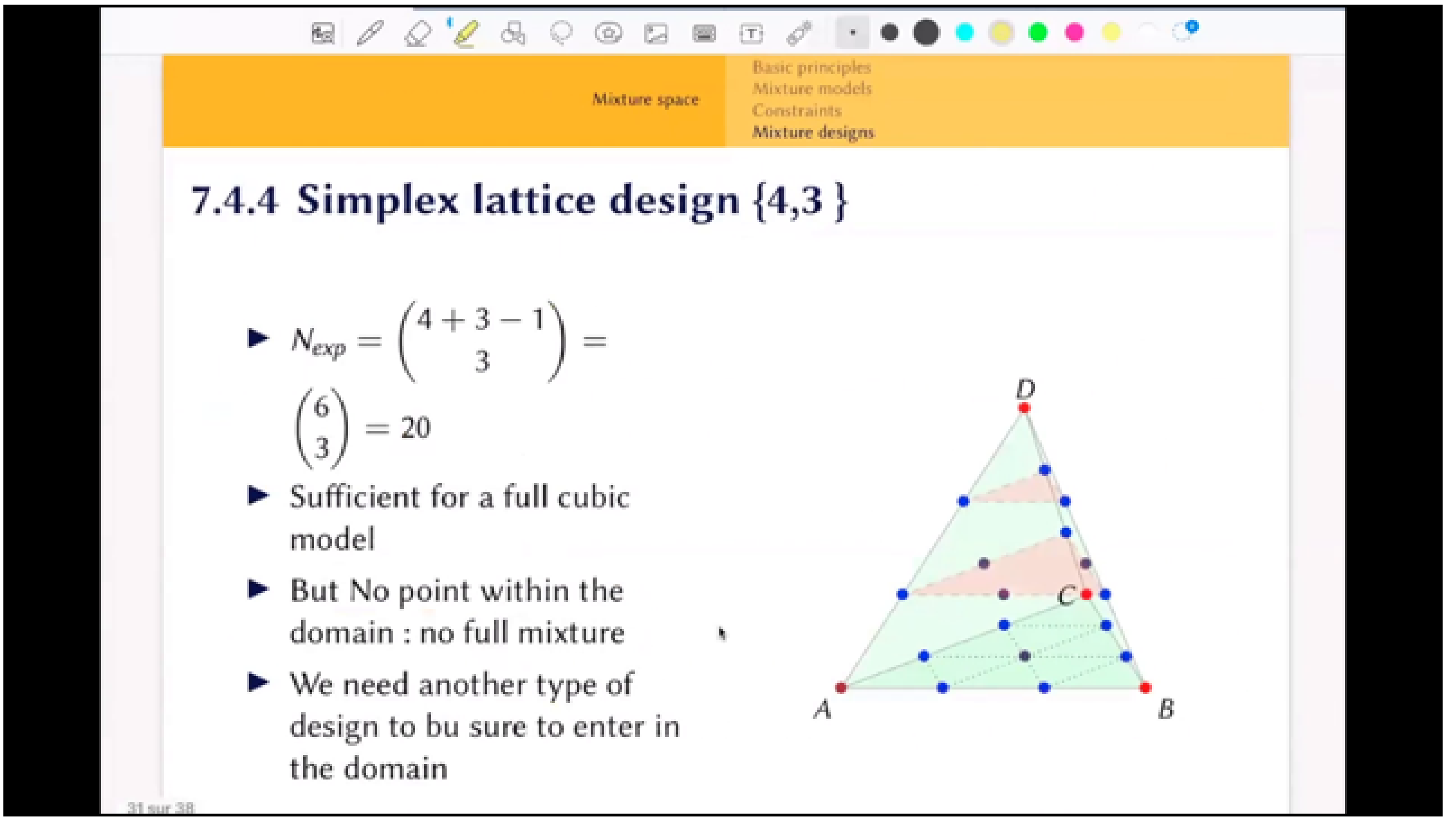


You can have sufficient numbers of degrees of freedom. Really, the only problem is what I mentioned you, that you have a lot of points that are single products or just small products. Here, I didn't calculate how many, but you can calculate the same calculation as I said before to understand how many points. So if you make this trick, I give you, you limitate your extension of all your products, 10% to 90% or I don't know 5%, 95%, you just decide what is good for you. You can use this type of design, simplex lattice design.

notes

summary

20m 25s

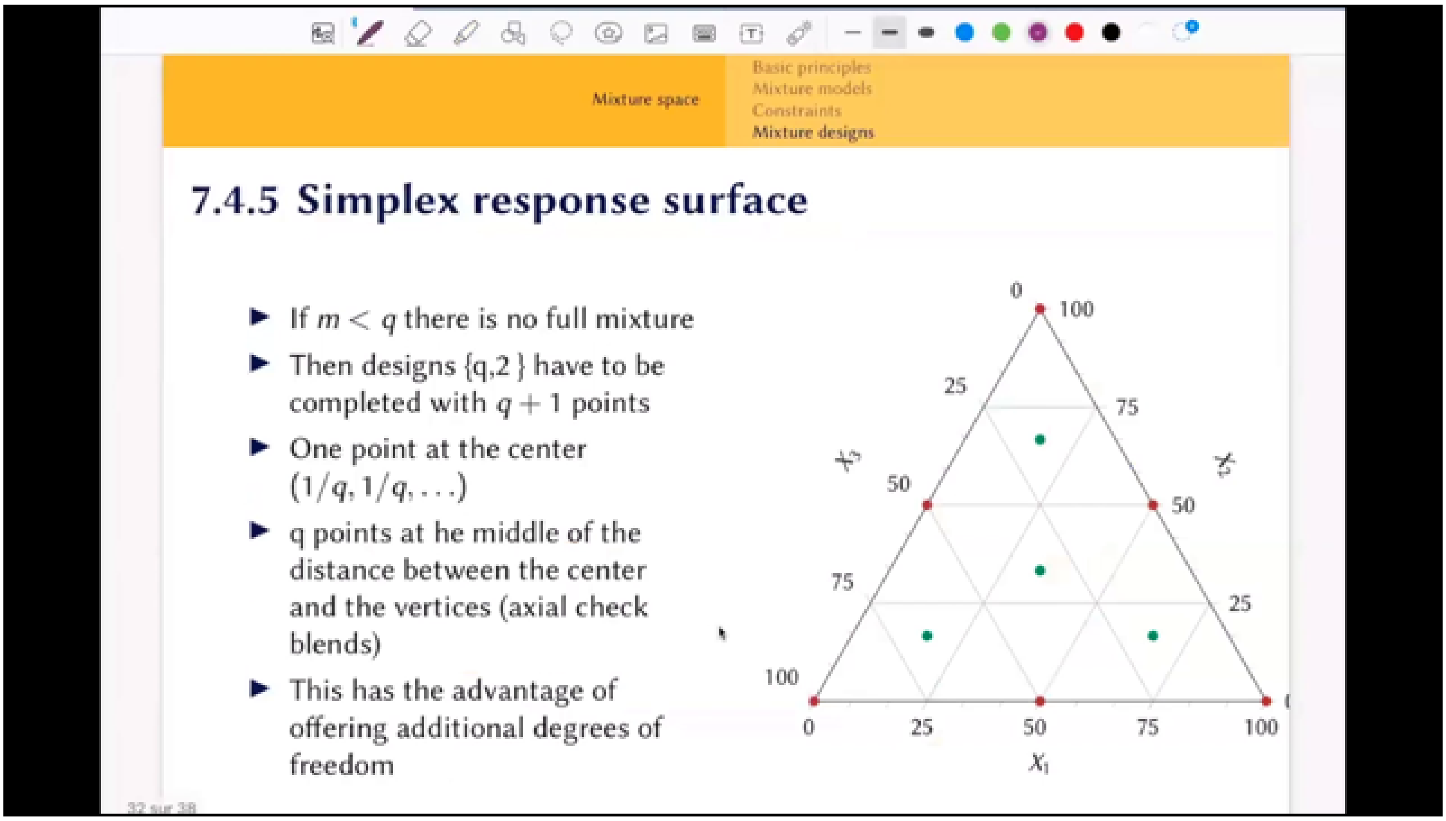


If the limit and the fact of having single product on only two products, only three products, experiment is not a problem. You see that with q equal 4m equal 2, you have sufficient degrees of freedom for filling a quadratic model in a four-dimension problem. But you see in this case that you have no full mixture, perhaps it's not a good solution. You have to use this trick of limiting my extension.

notes

summary

21m 9s

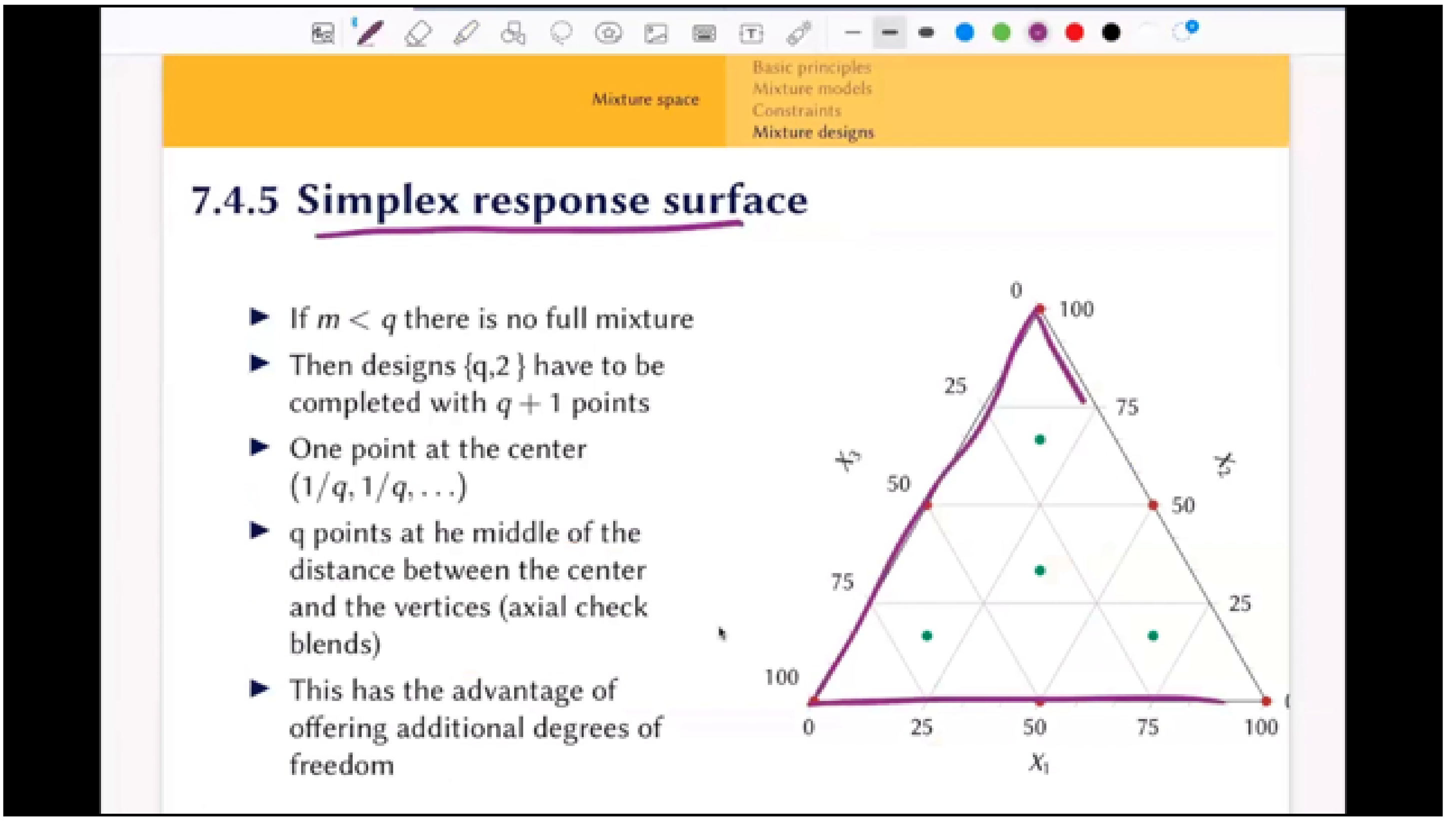


This was another example for three. I've calculated the number of point of experiment 20. So it's sufficient for a full cubic model. Again, no full mixture model. We need another type of design. This is the problem of the simplex lattice design is the problem of making too much experiment in a space which is not very adequate.

notes

summary

21m 40s

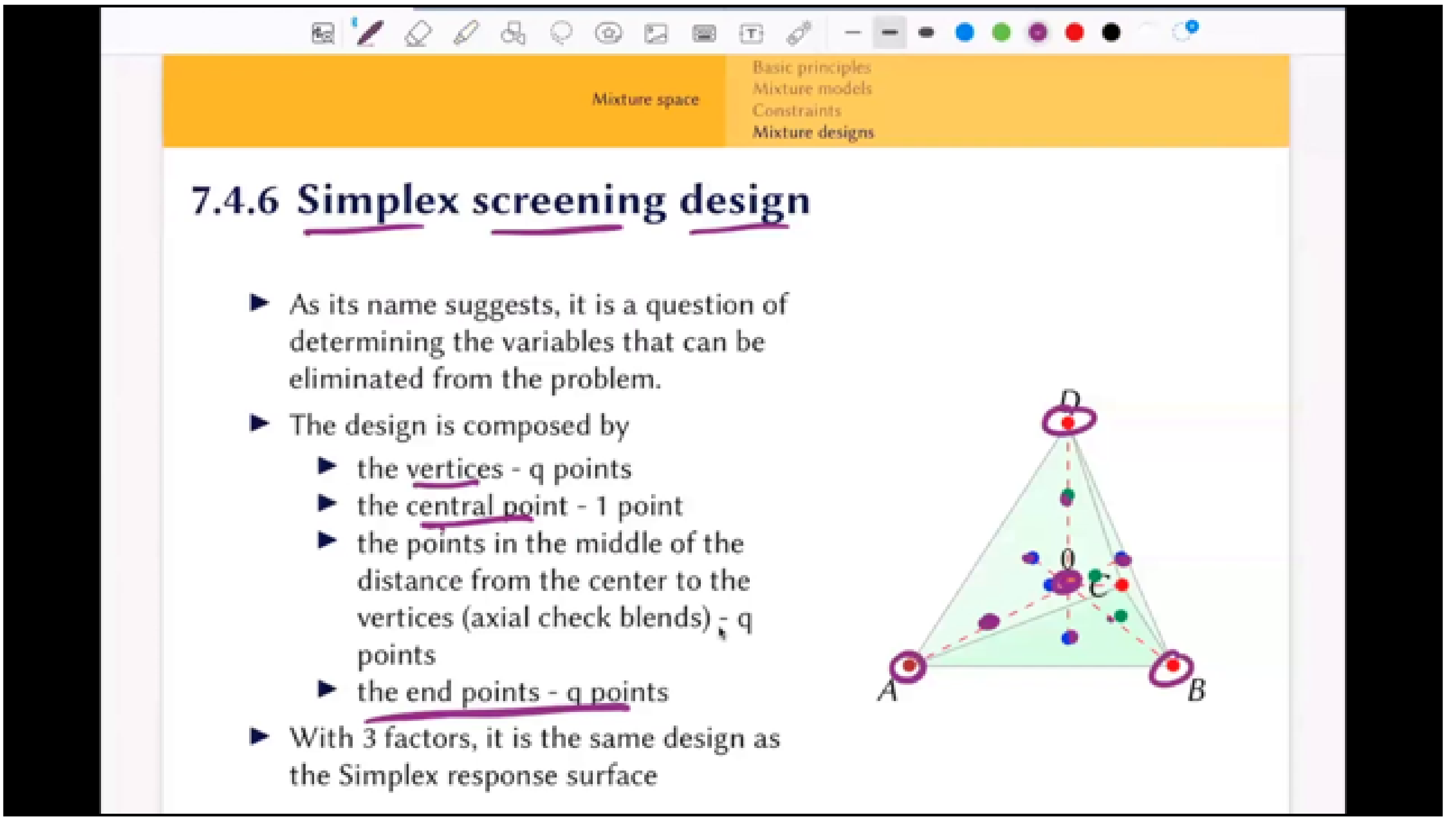


So we have something we call the simplex response surface.

notes

summary

22m 14s

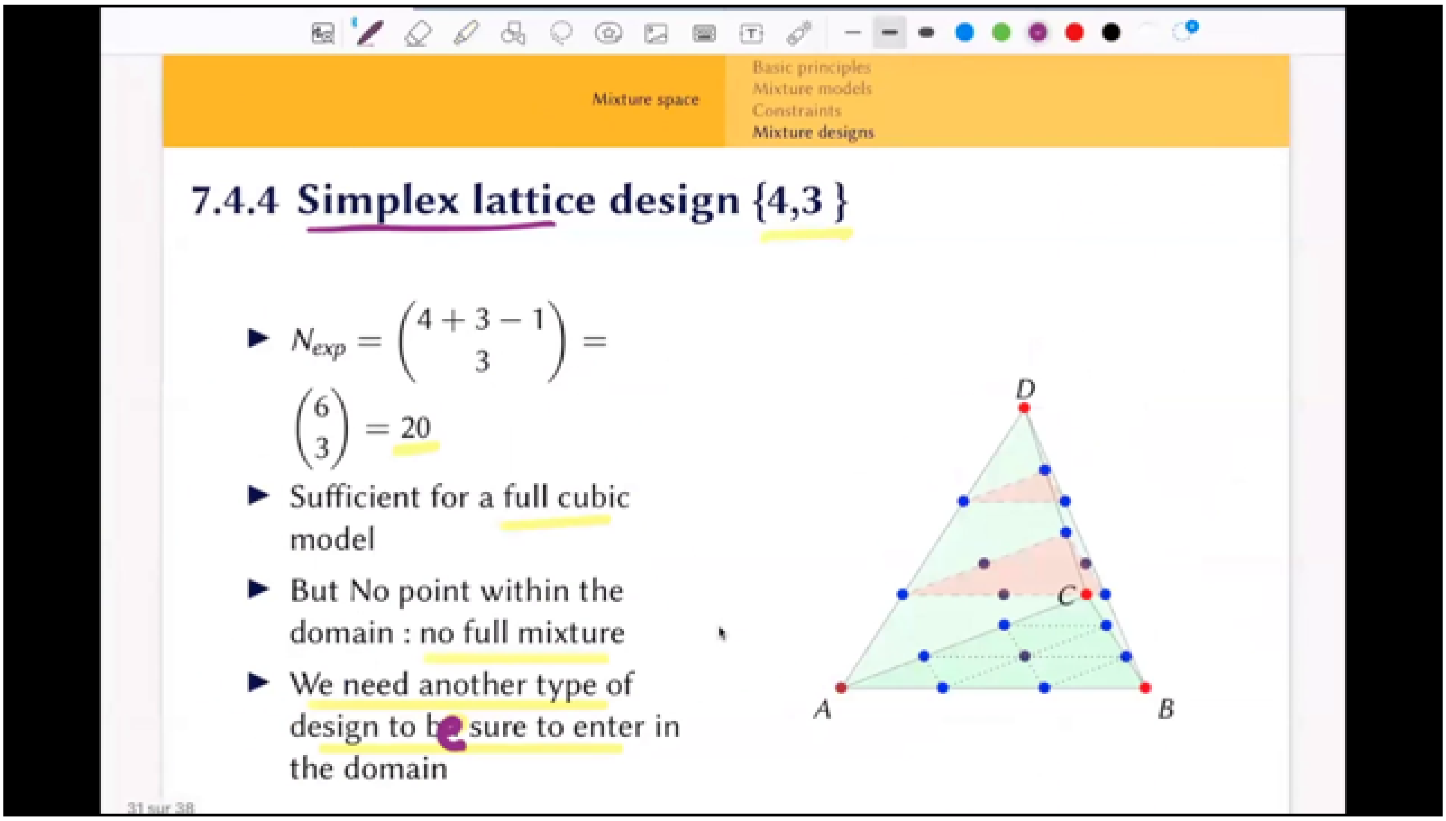


We still have the at the border, the points that we decide with the simplex lattice, but we had a few other points at the center of your domain and at the center between the center of the corner of the one of the corner, we make a point at the middle of that. And this is called the simplex response surface. So you see that in this chapter, let's say there are handmade designs, some ones are more efficient than others. You can do that. Personally, I would prefer the other strategy that I present to you before. And there it exists also another one called simplex screening design that you can use when you have a lot of factors and you want to screen them. So that means that you are in a first degree model. So you make points at all the summits. I made a central point here. I make points at the center of my face. So this was four products. And I'm also making movement points in the middle of the distance between the centers and the end point here.

notes

summary

22m 27s

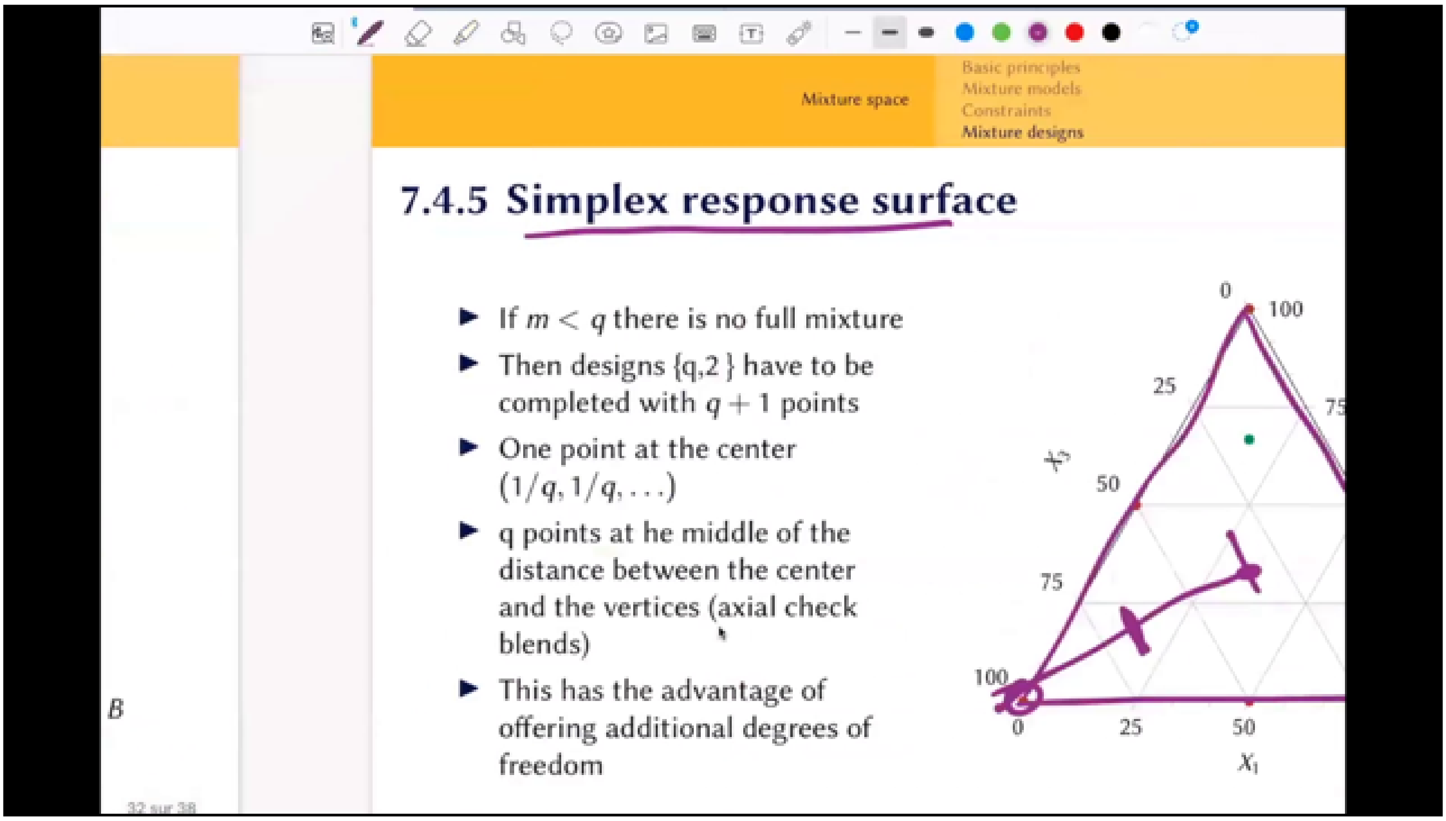


So we have three designs, simplex screening design, simplex response surface and simplex lattice design.

notes

summary

23m 49s

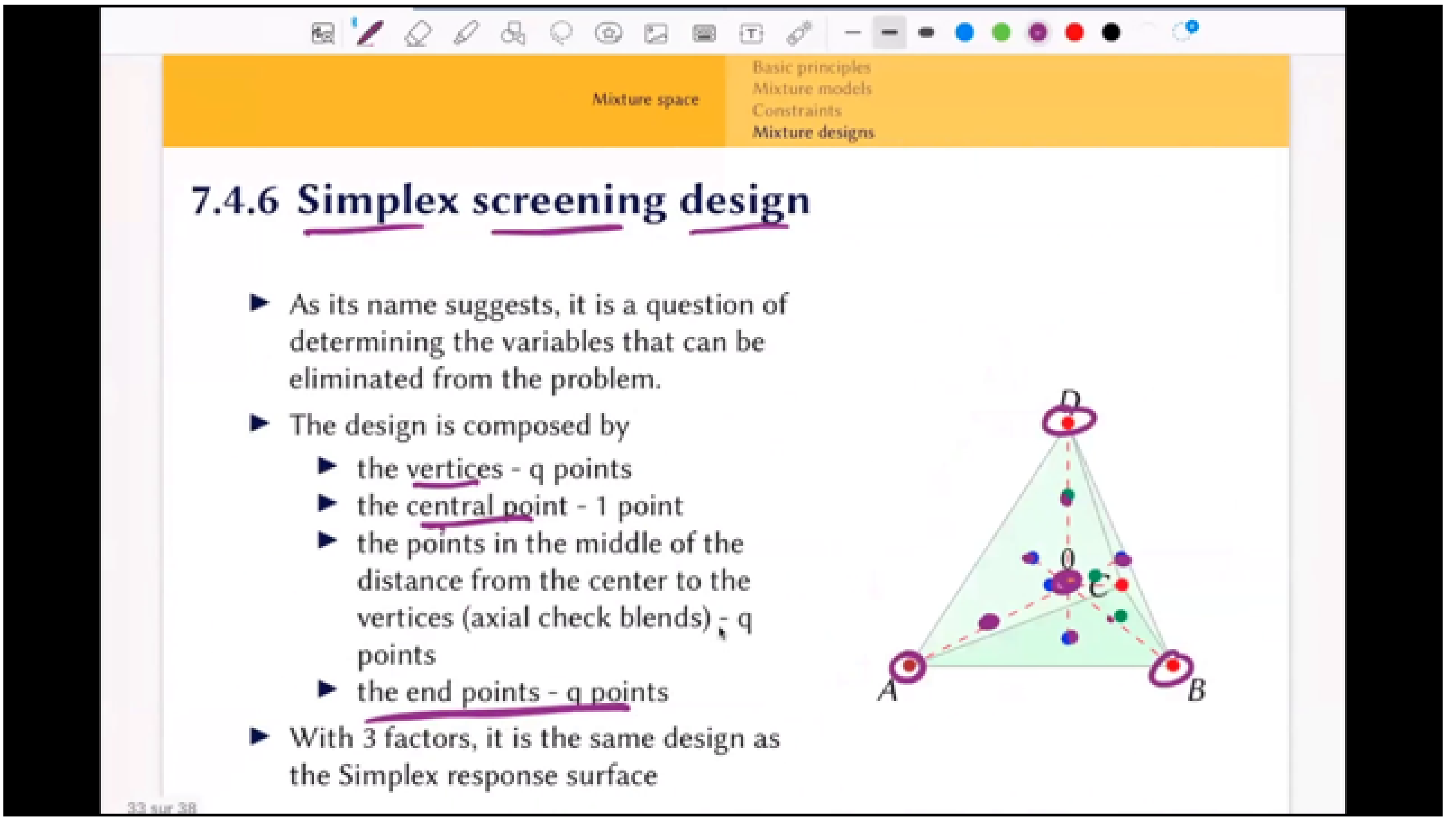


Simplex lattice is simple. The problem is the border, which is sometimes so nice. So I propose you a trick.

notes

summary

23m 57s

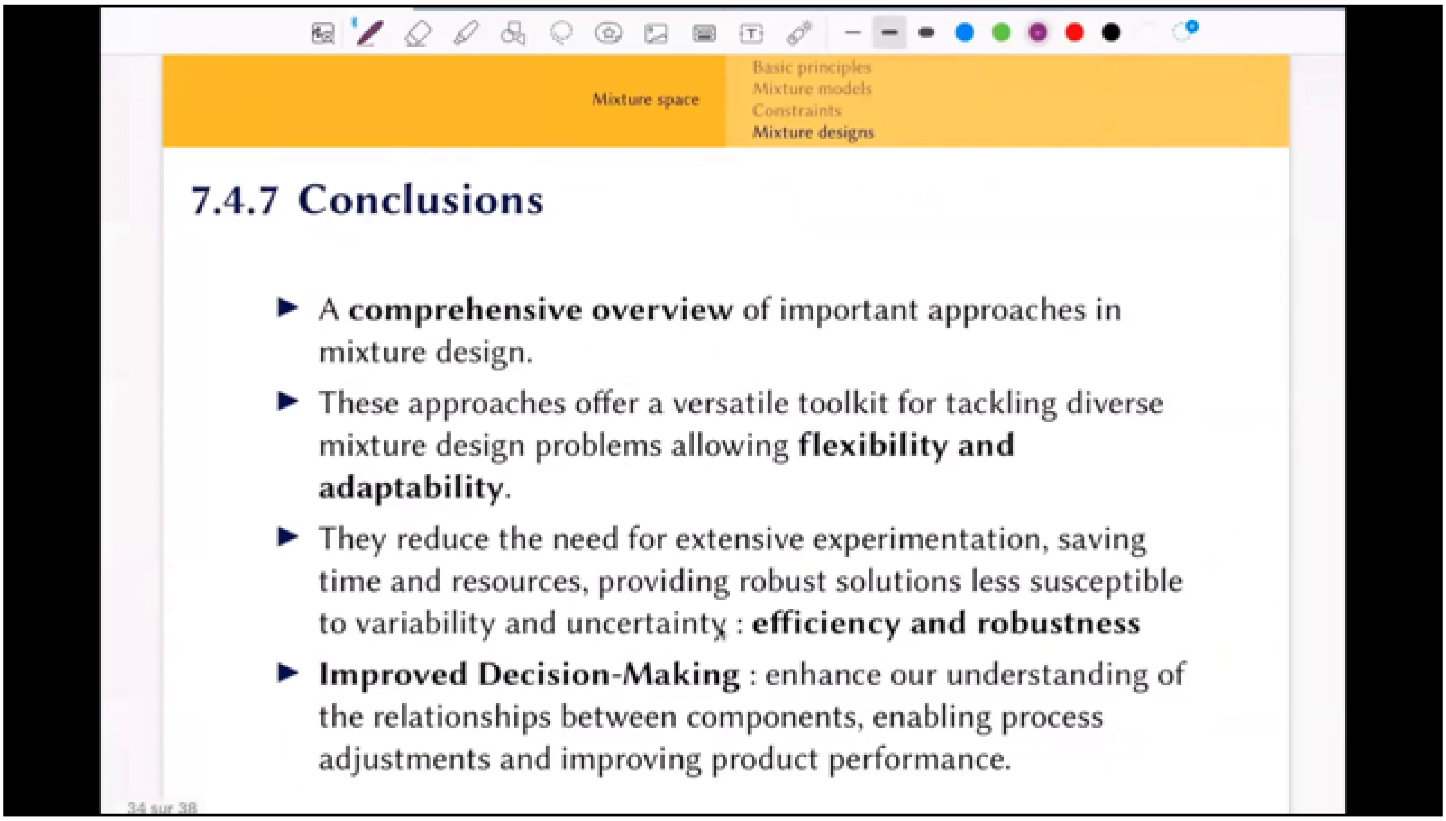


The simplex response is quite efficient. You still have a lot of points at the border. So this trick of limiting your surface to a limit of 10% to 90% could be quite also very nice to use.

notes

summary

24m 9s

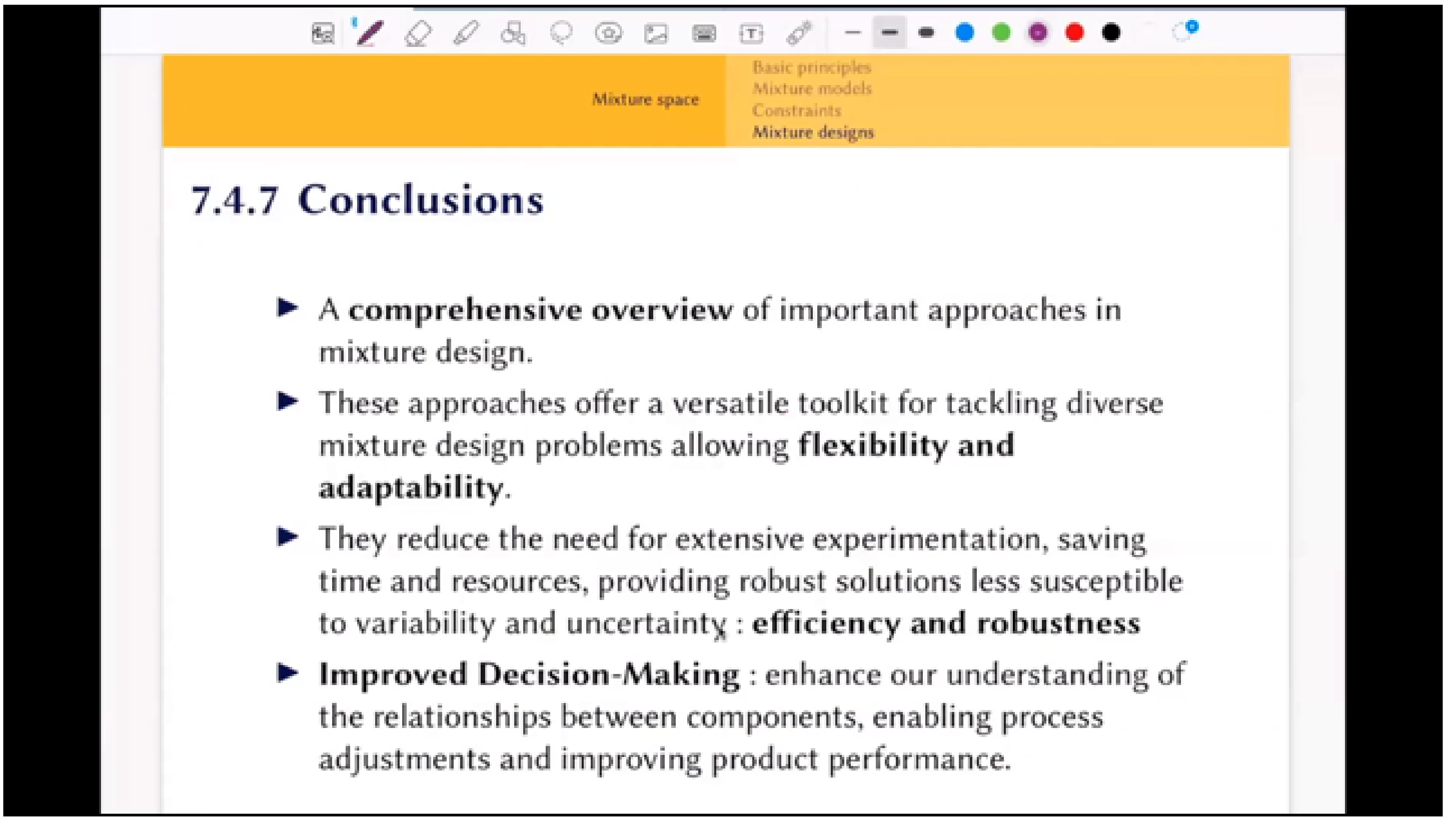


And after we have what we call the screening design, still have the problem of a lot of points are at mixture. So the tricky things in this type of design is that you want to be sure that what's happened when you have one of the products that is not present is critical or not. In some situation, it could be not critical. But if you are making a cake and you don't put eggs, it will not be a cake. Or you don't put sugar, it will be. So again, good structure, but you have to understand what you are doing and be on the void to apply those design just straightfully without thinking what you are doing.

notes

summary

24m 26s

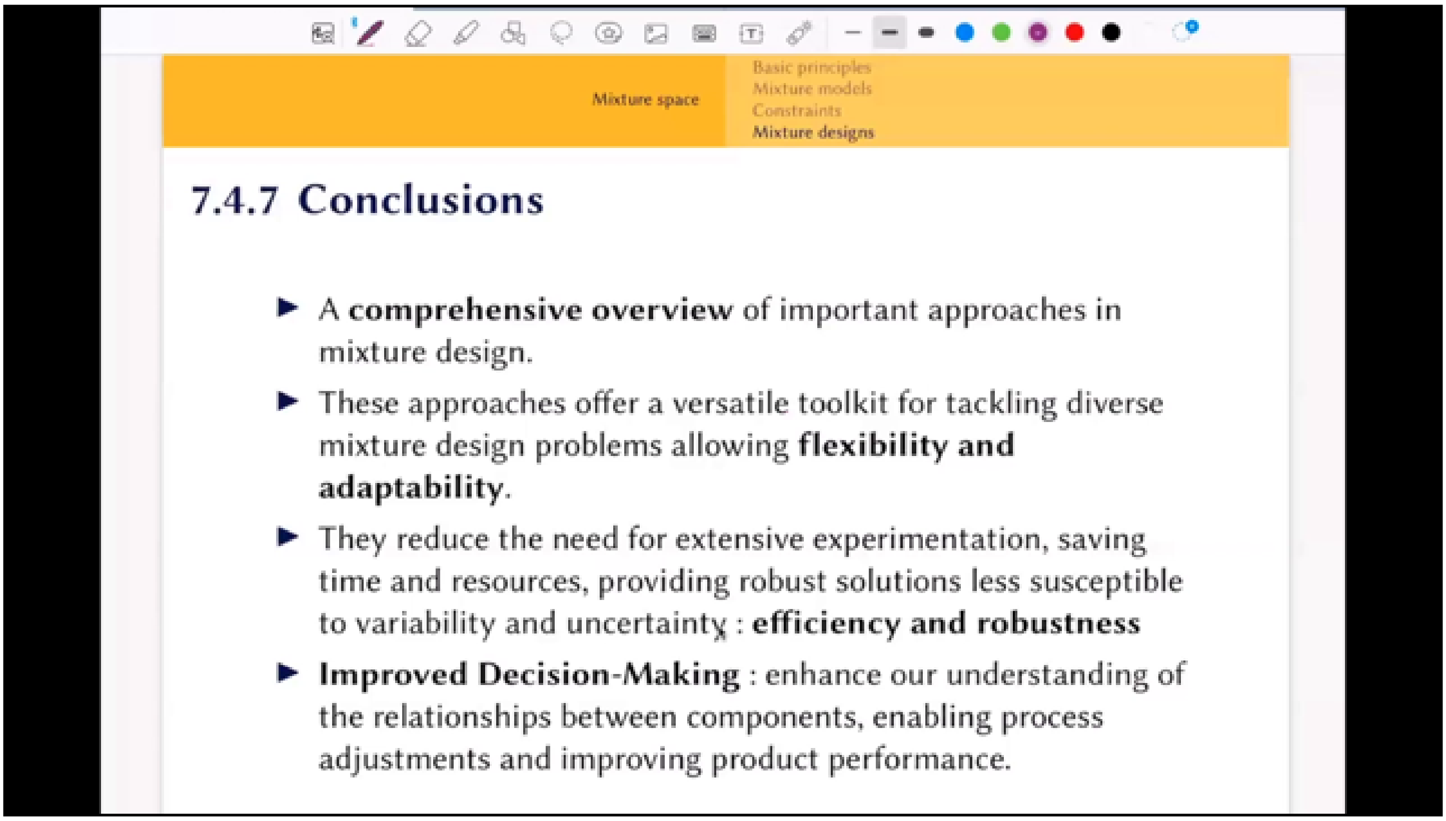


Okay, so I'm conscious that it was a little bit quick as a presentation is a, let's say it's more than a half chapter than than a chapter.

notes

summary

25m 9s



I'm not expecting you a full competency in this chapter. I'm just, I would like to understand the idea. You are able to understand the ternary graph because they are very important for making mixture and after understanding the philosophy. Or you are in a space which is still the original shape, a triangle, a pyramid or something like that. And you try to apply those classical mixture design. Or you are in a space which is because of the limitations that you have on not anymore, nothing to see with what could be a triangle or pyramid. And you try to use the standard design we have seen for the quadratic de l'art composite. You have to keep in mind that what you would like usually is flexibility and adaptability. You can have trouble to see all problems when you have a lot of dimension could be rapidly tricky. But mixture is the most tricky when you have more than three components. Slowly, step by step, understand that you will need perhaps more experiments that's a minimum because you really want to be sure. And in mixture, what really is important to be sure, the type of mixtures that you are doing, are you really visiting all the space or only limit because borders are all time complicated. But in mixture, they are even critical because it's natural mixture and eventually they do not belong to the space that interests you. Okay, so with this, I'm finishing with this chapter.

notes

summary

25m 18s