Course material

Course:

ENG606 / PHYS 442

Video:

DOE_lesson11_part2_ResponseSurface

Concepts (extracted from automatically generated subtitles):

Maximum value. Dispersion matrix. Root mean square of the results. First thing. Center of the body. Minimum value. Power k. Second degree. Linear coefficient. View of the dispersion matrix. Case of the delert. Little bit. Quadratic model. Interesting things. Contour line.

to video sequence search
(within ENG606 / PHYS 442.)

to video

Center for Digital Education. More educational support material here:
https://www.epfl.ch/education/educational-initiatives/cede/educational-technologies-gallery/boocs-en/

...

notes

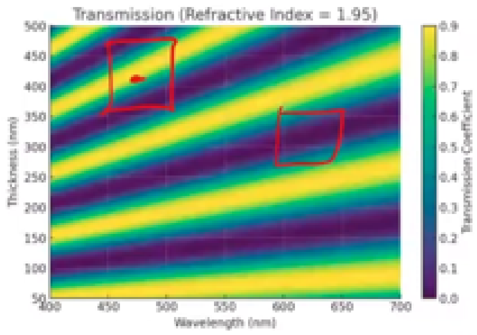
summary

0m 0s

5.2.13 Application : light transmission

- The transmission or reflection of light by a thin film is a complex phenomenon.
- Based on Snell and Fresnel equations, for a perpendicular non-polarized beam, the transmission coefficient T giving the fraction of intensity which is transmitted is function of the wave length λ, of the refractive index n and the film thickness t such as

$$T = \left(1-\left(\frac{n-1}{n+1}\right)^2\right)\sin^2\left(\frac{2\pi n t}{\lambda}\right)$$



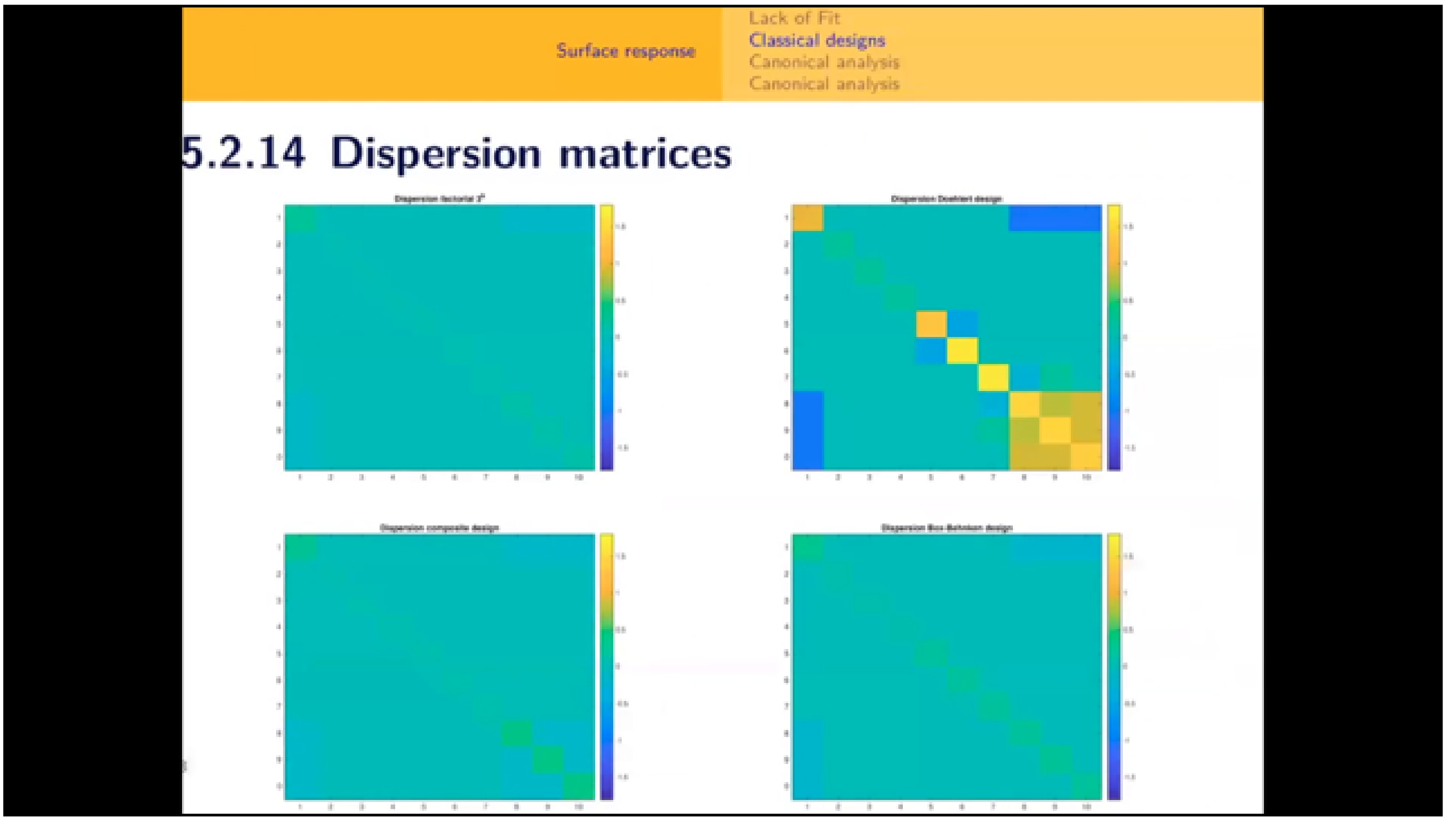
- The objective is to experimentally determine R around the point ($\lambda = 475\ nm(blue)$, $t = 425\ nm$, $n = 1.95$)

These subtitles have been generated automatically So what I did yesterday, I take this function and I simulate an experiment.

notes

summary

0m 1s

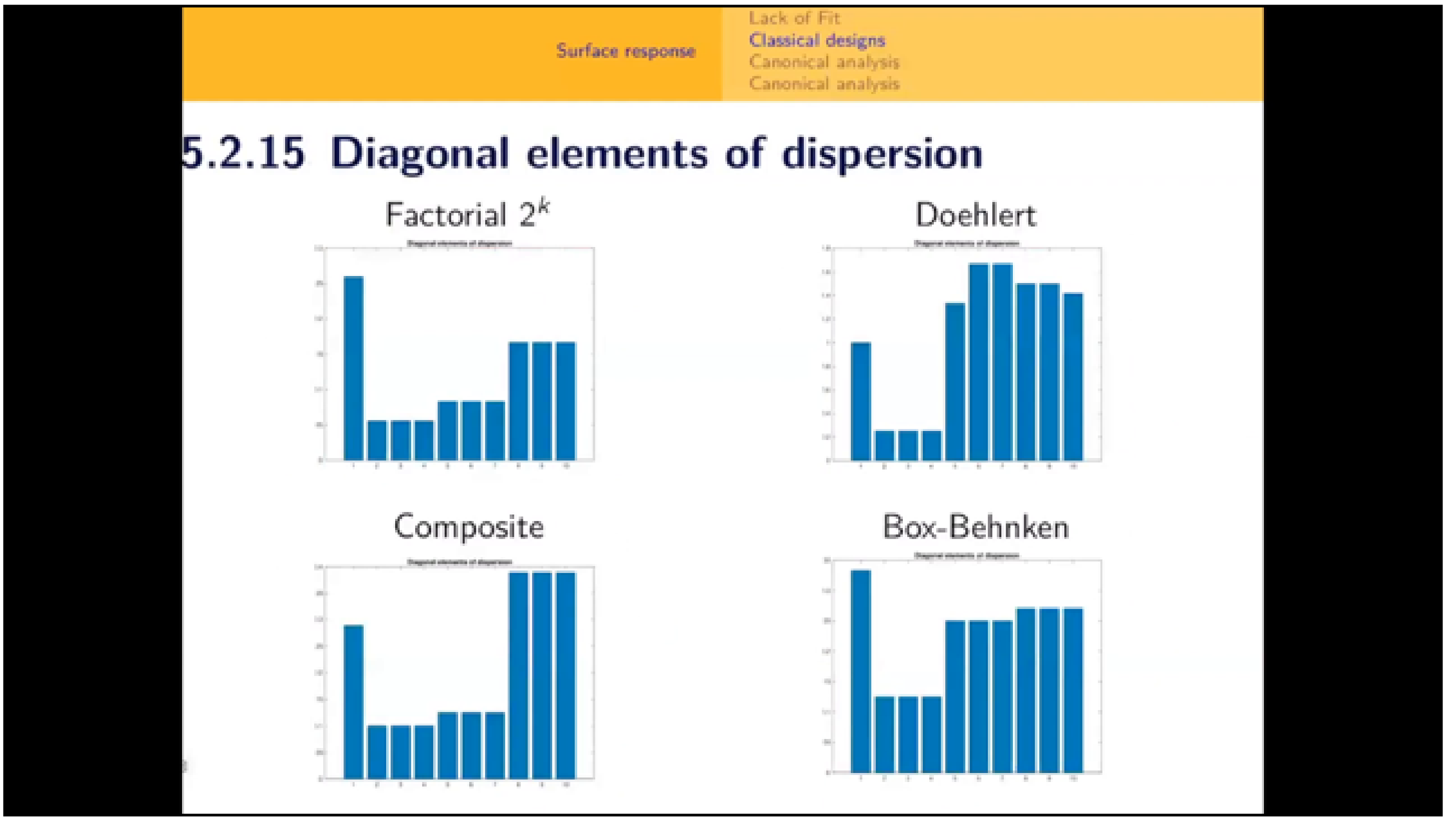


So it was very easy for me to simulate the experiment. I take this function and I add a noise, a random noise to it for making, okay. But the idea would be we would like to make a model, a quadratic model of one of those frames around the points 475 for the wavelengths, 425 for the dimension of the film, and 1.95 for the refractive coefficient. And so I did it.

notes

summary

0m 5s



It was, it took time, but it was easy. I did it with the four design I present to you. So the first thing was to calculate the, the, the dispersion matrix. So this is the view of the dispersion matrix. They are all the same cod of color. If you don't know how to do it, you can use say limb. So you can impose in those maps, you can impose what is the maximum value, what is the minimum value for having maps that you can compare. And you have the three power K here. I have the composite here. I have the dollar here and I have the box bank in here. So you see that the three, the 3K composite and the box have qualities that are very, very alike. Except that 3K costs quite the double of the other. You have 27 experiments when here I have a composite, I have 15 and here I have 30. So you see it's very typical of the quadratic. So the quadratic dispersion matrix is more easy to see in the delert because it's very typical. You have values and the diagonal and the minimum, minimum is you have aliases between the quadratic and the constant. This is very typical matrix for the second degree. But in the case of the delert, you see that I have some other problem. The delert is also 13 runs, but the quality is a lot worse than the other. So in this case, if you have to choose, I would say I will choose box if money is very important. I will choose the composite if I want to make a balance between the numbers of run and the quality. There are other aspects that we will see later and I will choose 3K if I'm very rich and I want to make a lot of experiments. So a first view,

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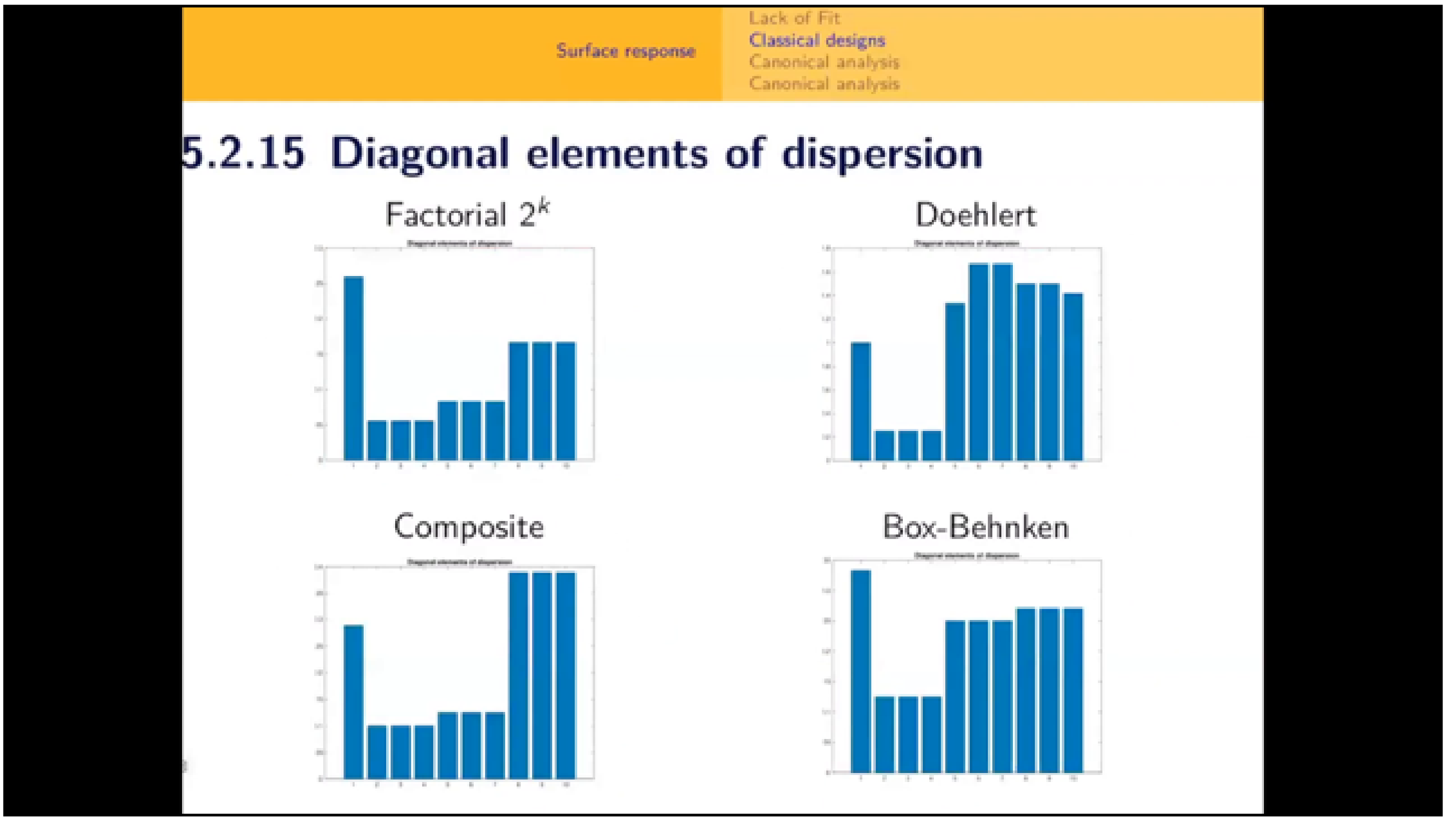
0m 47s



a first comparison of this four design. Again, delert is interesting, it's cheap, its quality is quite low. Remember that.

notes

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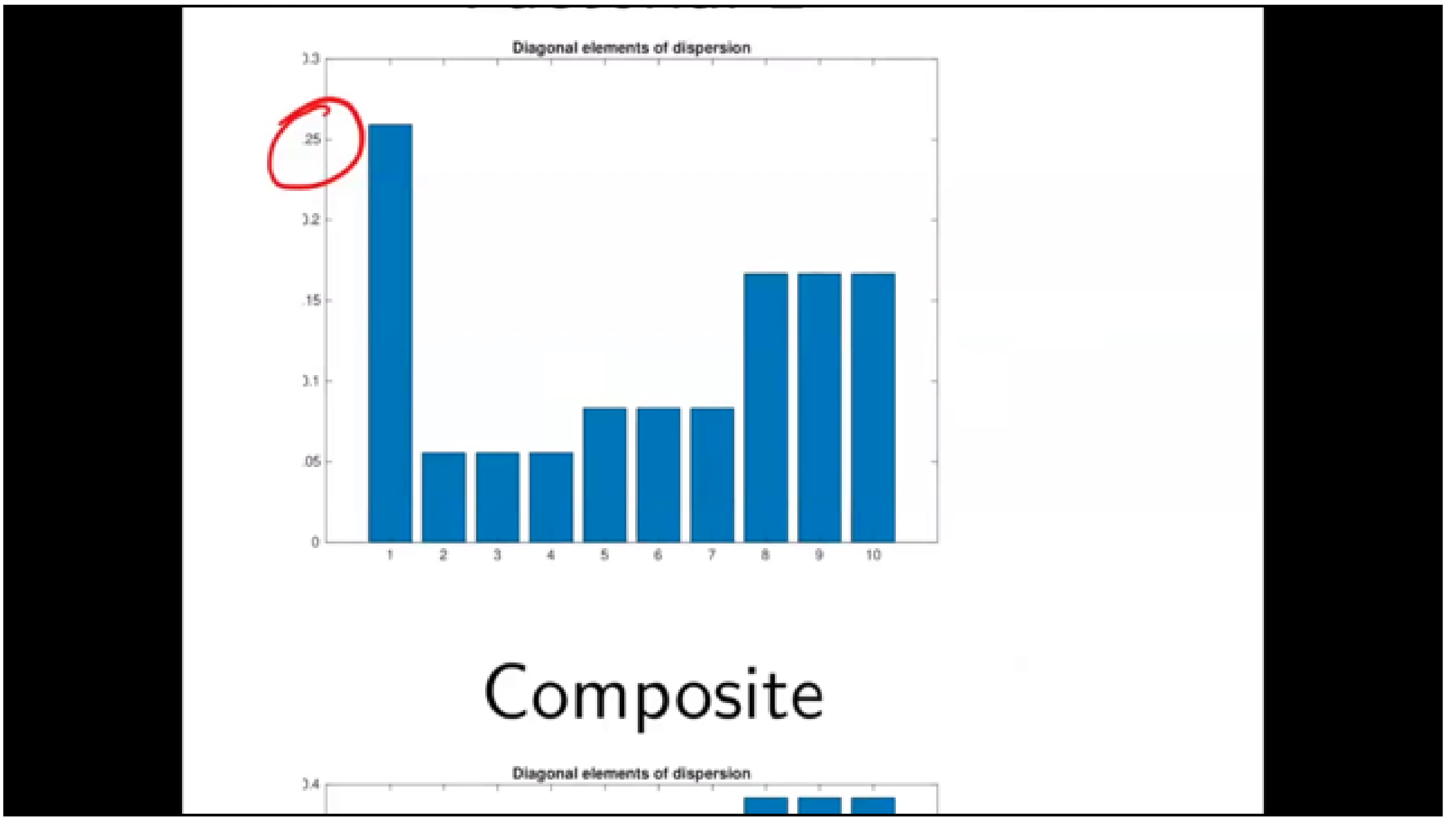

After I have looked at the diagonal element of the dispersion matrix. So it's quite the same information, but it's just the diagonal of my picture before. You see also the value. So you see that I have something as 0.25 for the 3K for the constant. And after I'm around, what is the value? Yes, 0.15, 0.10. That means that I'm recuperating something as between 10 and 15% of my experimental error on my coefficients.

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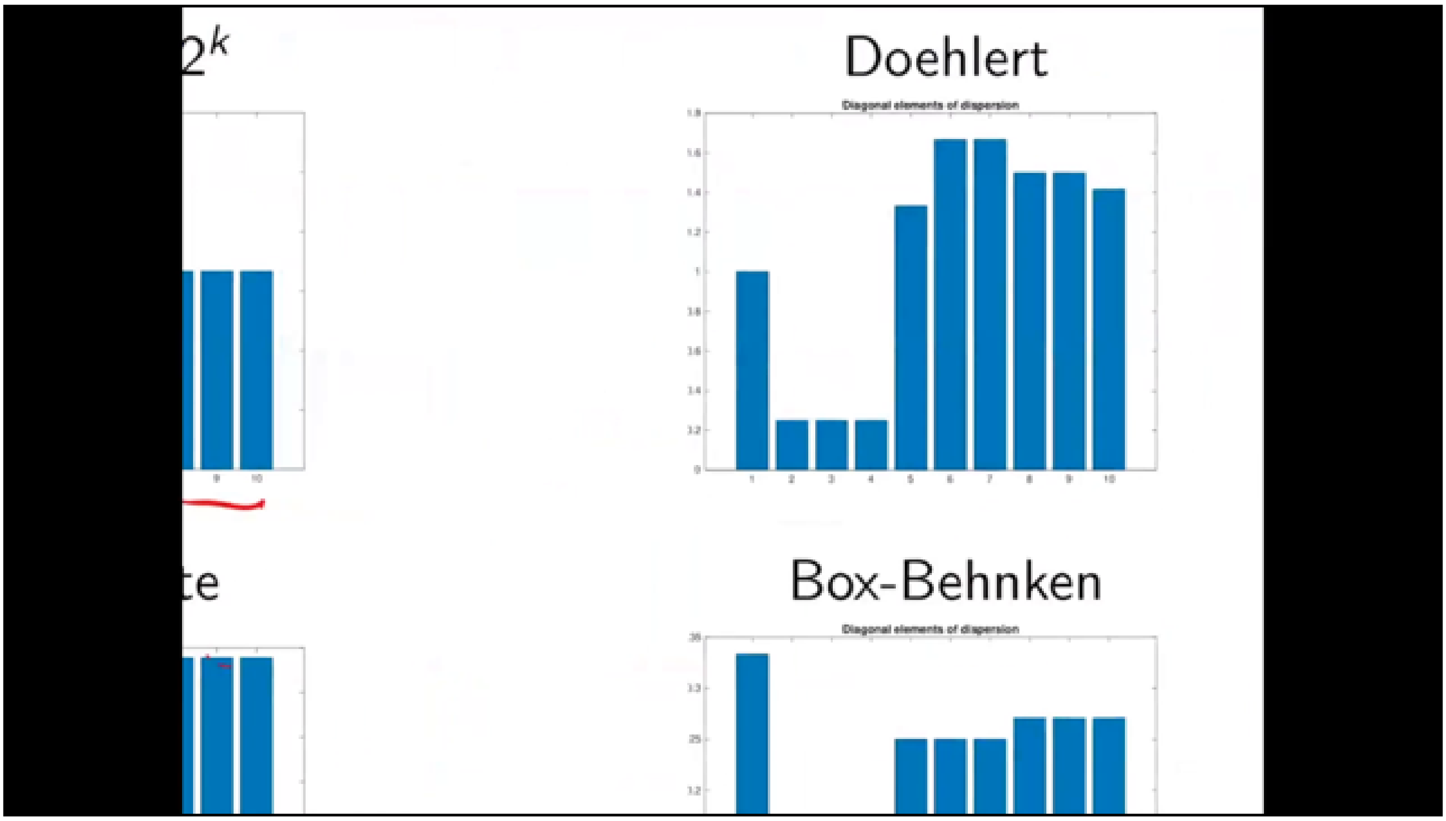
summary

3m 28s

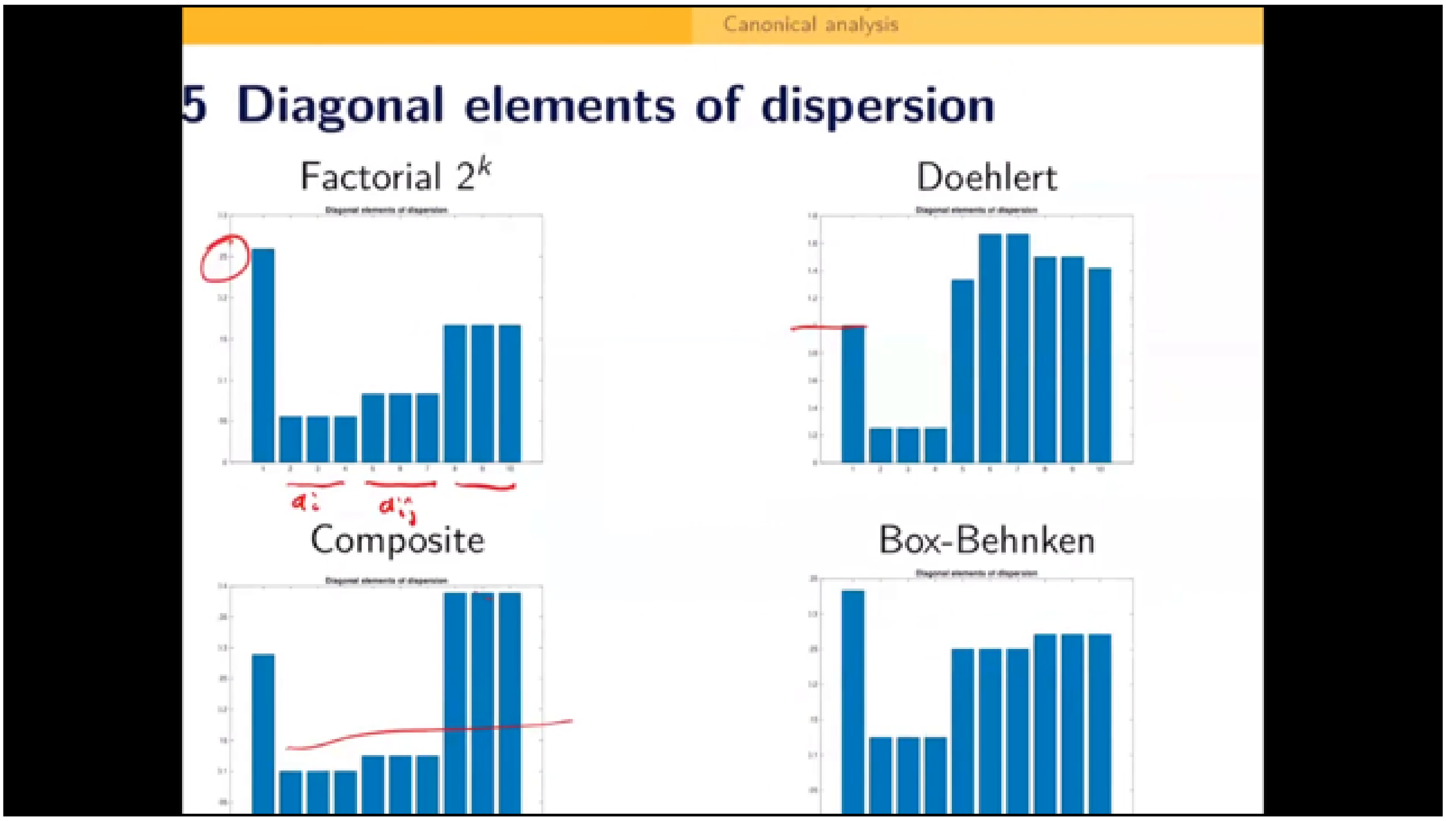


Quite good. You see in the composite that those values are quite the same for the worst case and 10% a little more than 10% for the linear coefficient and the interaction. Sorry, I didn't explain. So very well, you understand that this is the value of the diagonal for each of the coefficients. So the first one is the constant after I have the three linear, this is the IE. These are the three interactions, A, E, G, and those are the quadratic terms.

notes

summary

4m 13s

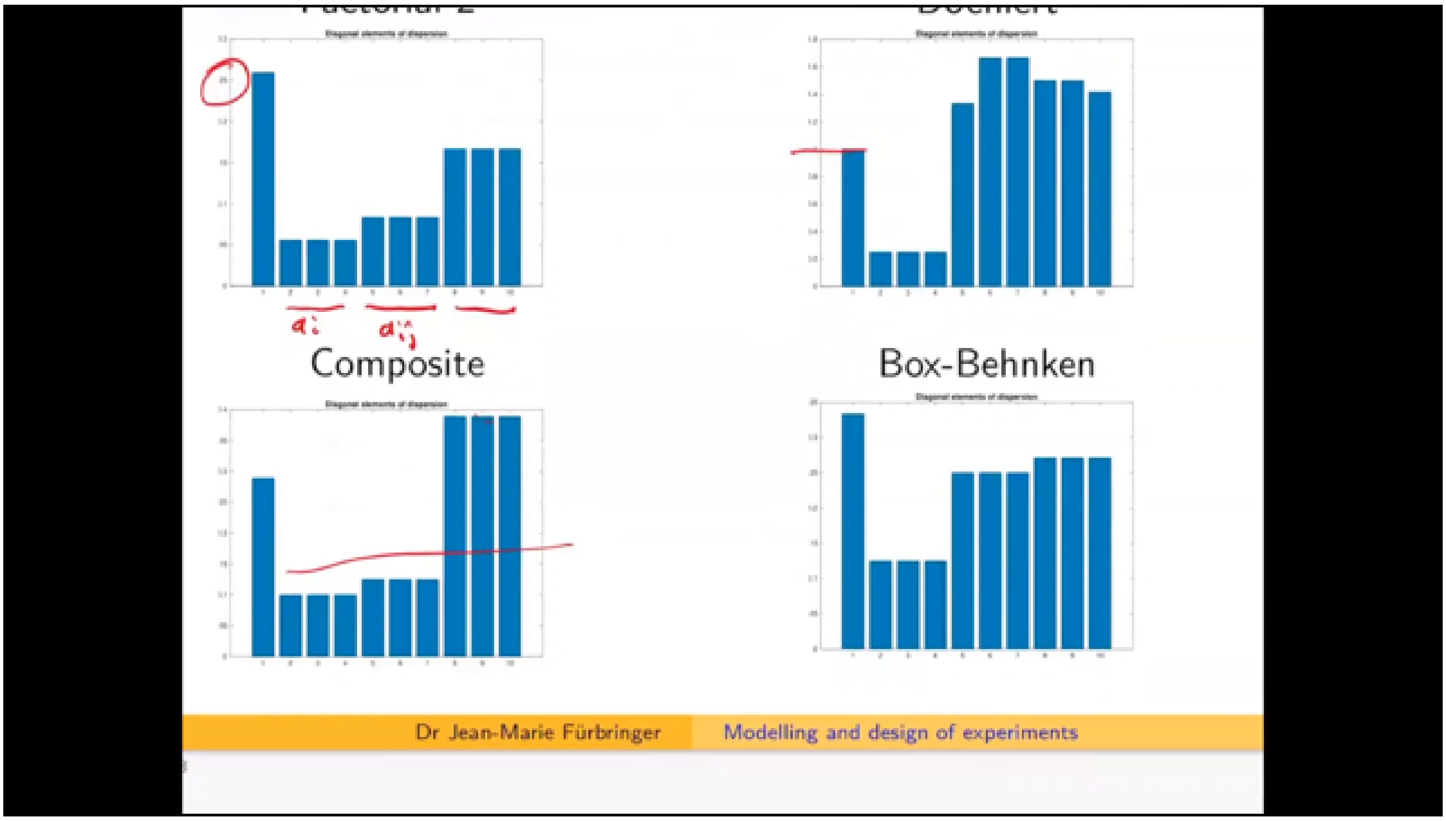


After you see the dollar, that's really you see here that the value of the dollar is confirmed what we already see. We see that for the constant, we have 100%. And even for the interaction and for the quadratic terms, we have 60% more of accuracy of inaccuracy than the other. So I'm multiplying the uncertainty by 1.5, 1.6 is what I said is a very cheap design. It's very practical, but it's very cheap. So you have to remember to remember that.

notes

summary

4m 55s



So that means that it works quite well when you have very precise measurements in situations where your measurements are not very precise. So if you have 1, 2% of error in the measurement, it's quite okay. You will have the double of it on your coefficients. 2% of error in your coefficient is not so bad. But if you have 10% of error in your measurements, it's become quite complicated and you better avoid this type of.

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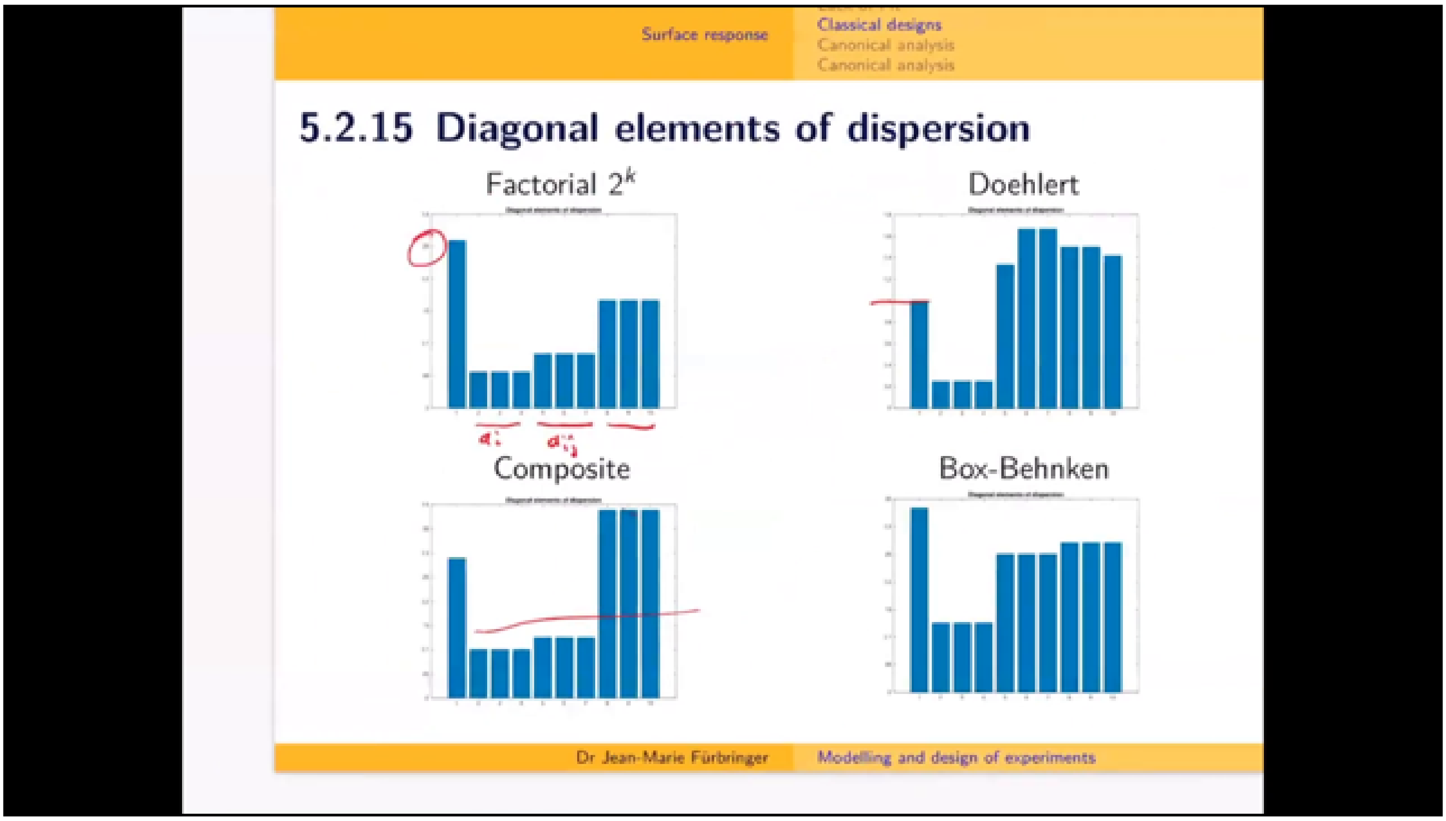
5m 37s



And BoxBencken is also quite a good design.

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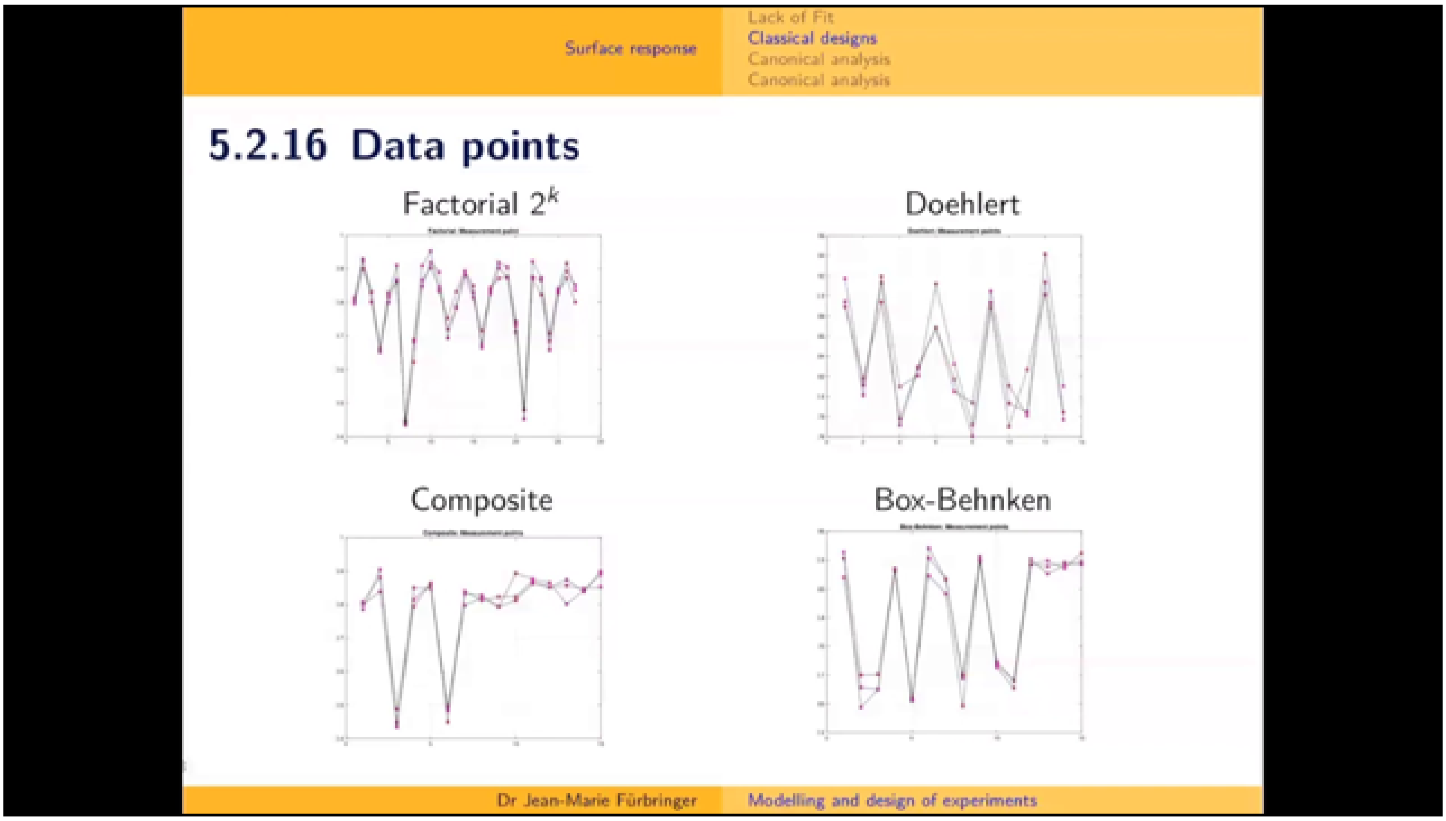
6m 13s



So what you see here with the numbers, it's before in this, it was more of a structure. You see the color, it was more of a structure. You see here the values, but it's quite the same information. You see that again, okay, if you have very precise measurement and you are interested by his features, you want to move or you want to increase the numbers of factors and things like that. But the part of that is not a so good design. After is the price of your design that will make the difference because the quality is interesting. The quality of the factorial 3k is not so much better than the other. I'm making the double of experiment, but in fact, I'm not gaining so much. So this is my simulation.

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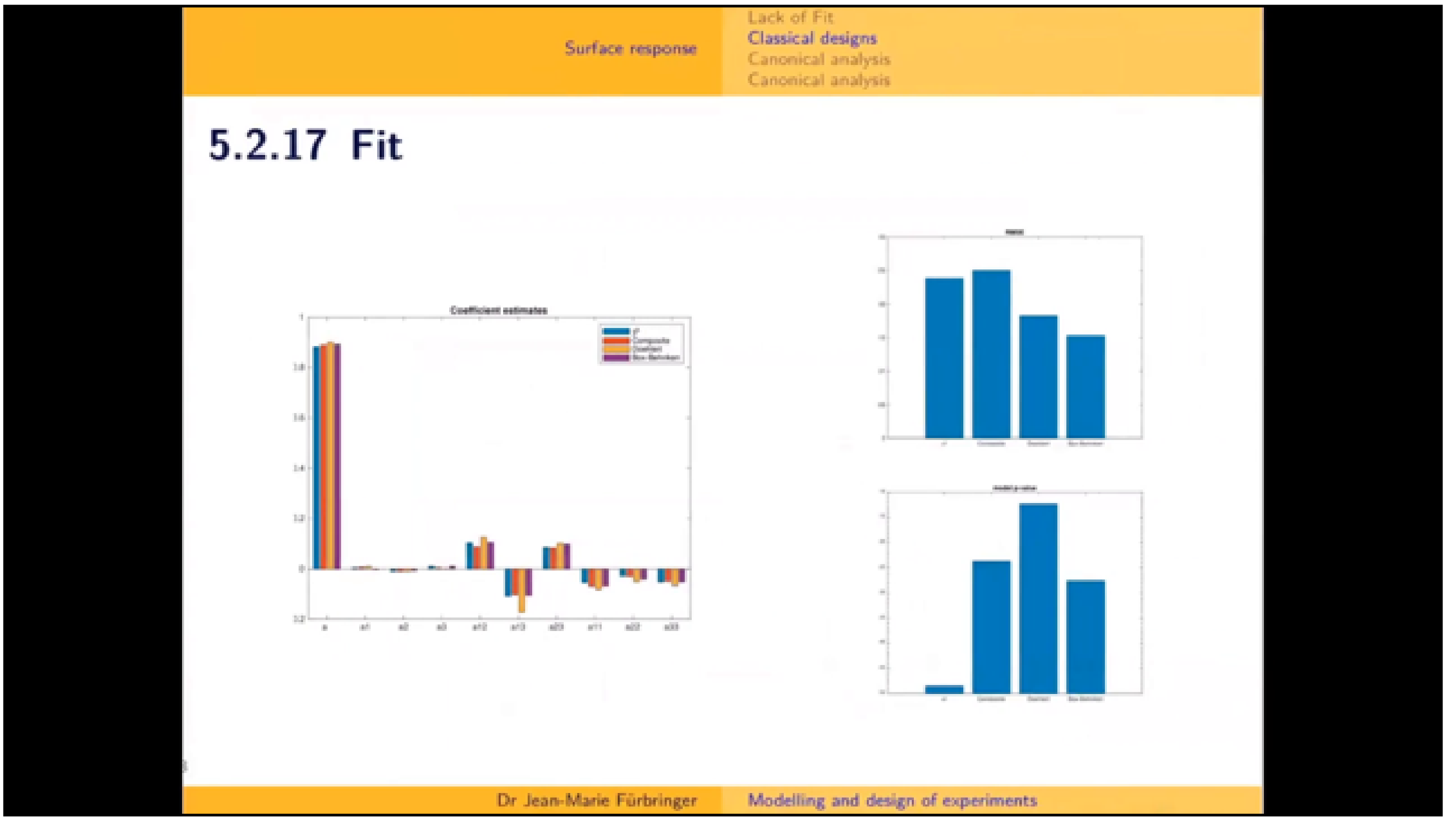
6m 15s



So it was just the use of my model plus some noise. Okay, just for showing you that I'm making my job correctly. It's not interesting things to discover in that.

notes

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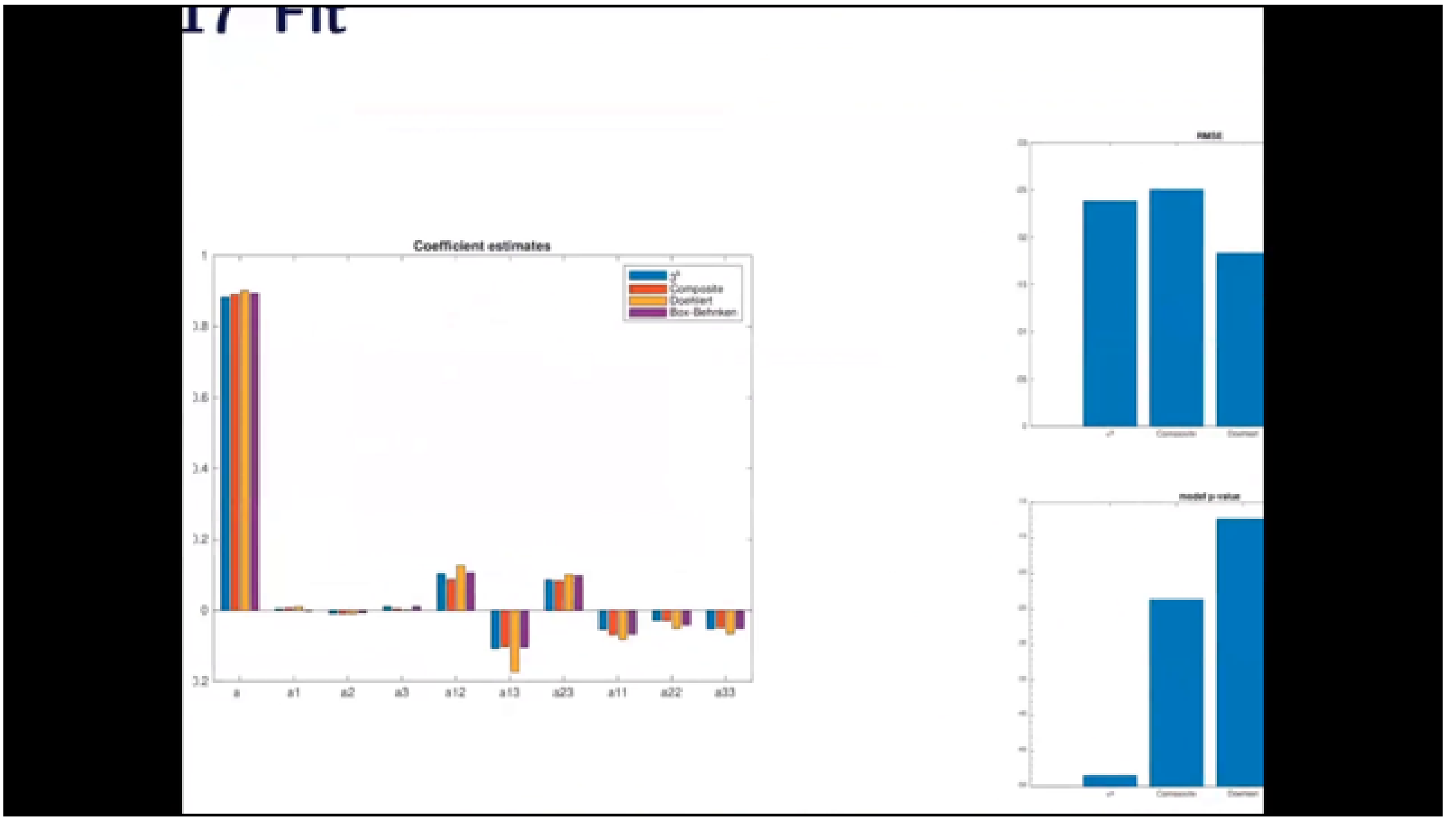
7m 3s



Remember that when you execute a design, never execute it in the way you generate it. Usually you generate it so very regularly and after use random choice of experiments for realizing it because you want to avoid to have aliases with your practice of experiment. So now I have made the fit. So I make this simulation and I made the fit for each one.

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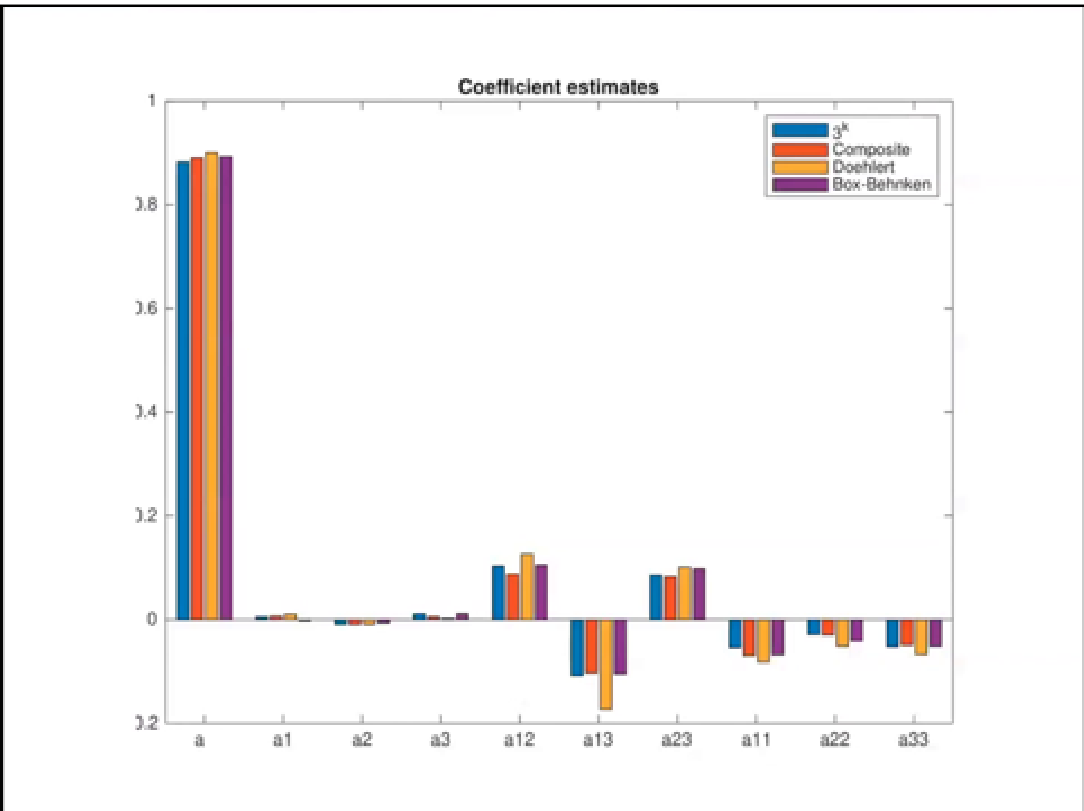
summary

7m 19s



So if you look, okay, we get things quite the same. So I have not cheat, but I have play a little bit with the numbers with this because, okay, you see my function was pretty quite a square sinus. So if I make my range a little bit too large, it was going up. So I have restrict quite a lot my design. I have used my composites.

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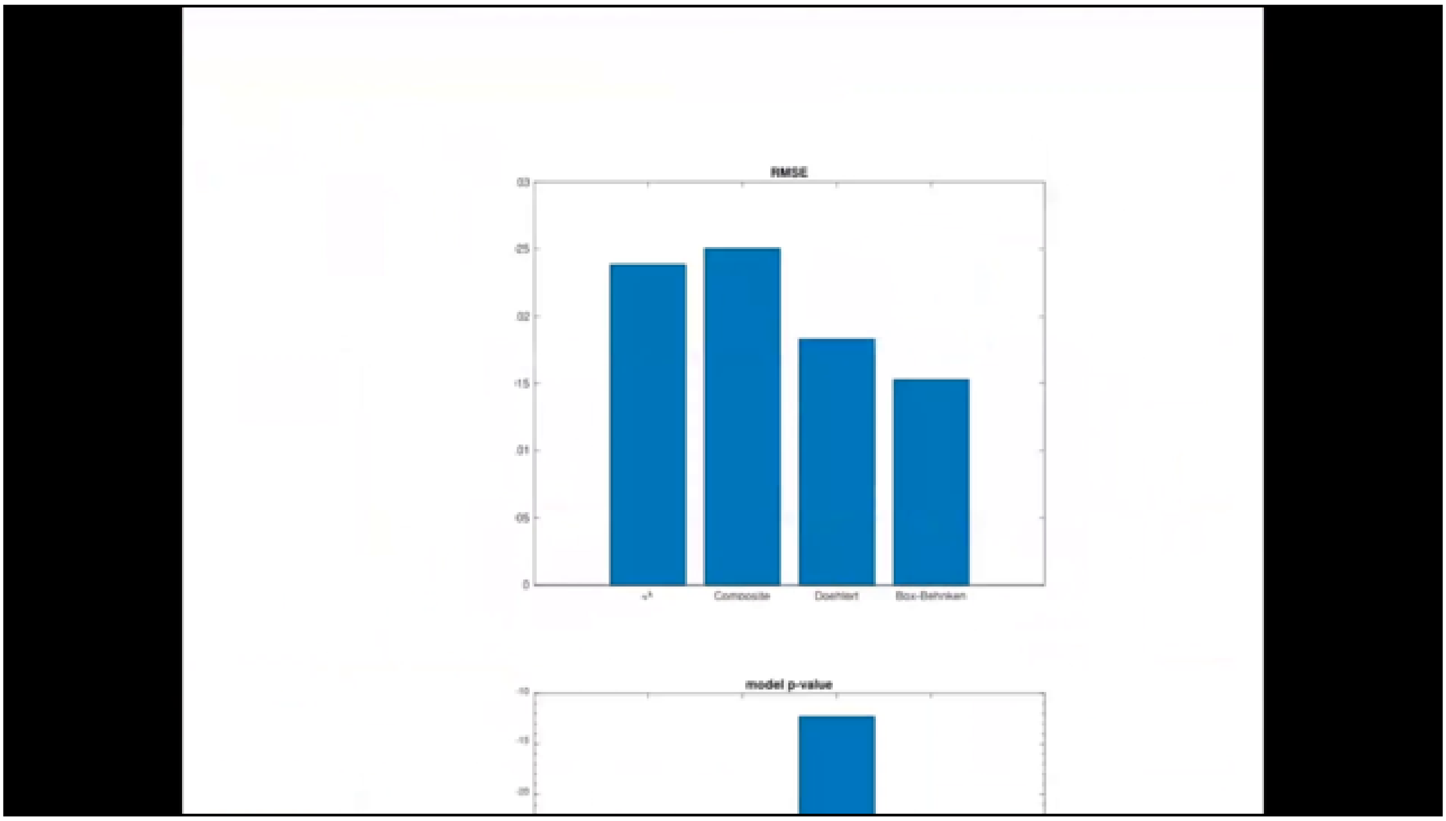
summary

7m 50s



I have also make the alpha value one for not going more away than the other. And you see that the results, well, they are very comparable for the constant. In our model, we see that I quite have no linear effect. And for the interaction and the quadratic, I have things that are comparables are not exactly the same. You see that really the delert, the yellow one is each time aside of the other, but they quite all make the job quite correctly.

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8m 25s

And now I have checked the root mean square error. That means so the root mean square of the results, the variance, putting all together the lack of fit and the pure error. And again, you see that those values are comparable. And now after I discover the P values. Okay, so here you have your investment back. You see that the three power K that is making the double of experiments as higher, lower, sorry, as lower P value is definitely better. Is where where the effort that you make making the double of experiment is really bringing the difference. And after you see that the dollar is definitely the worst, but not so bad than the other.

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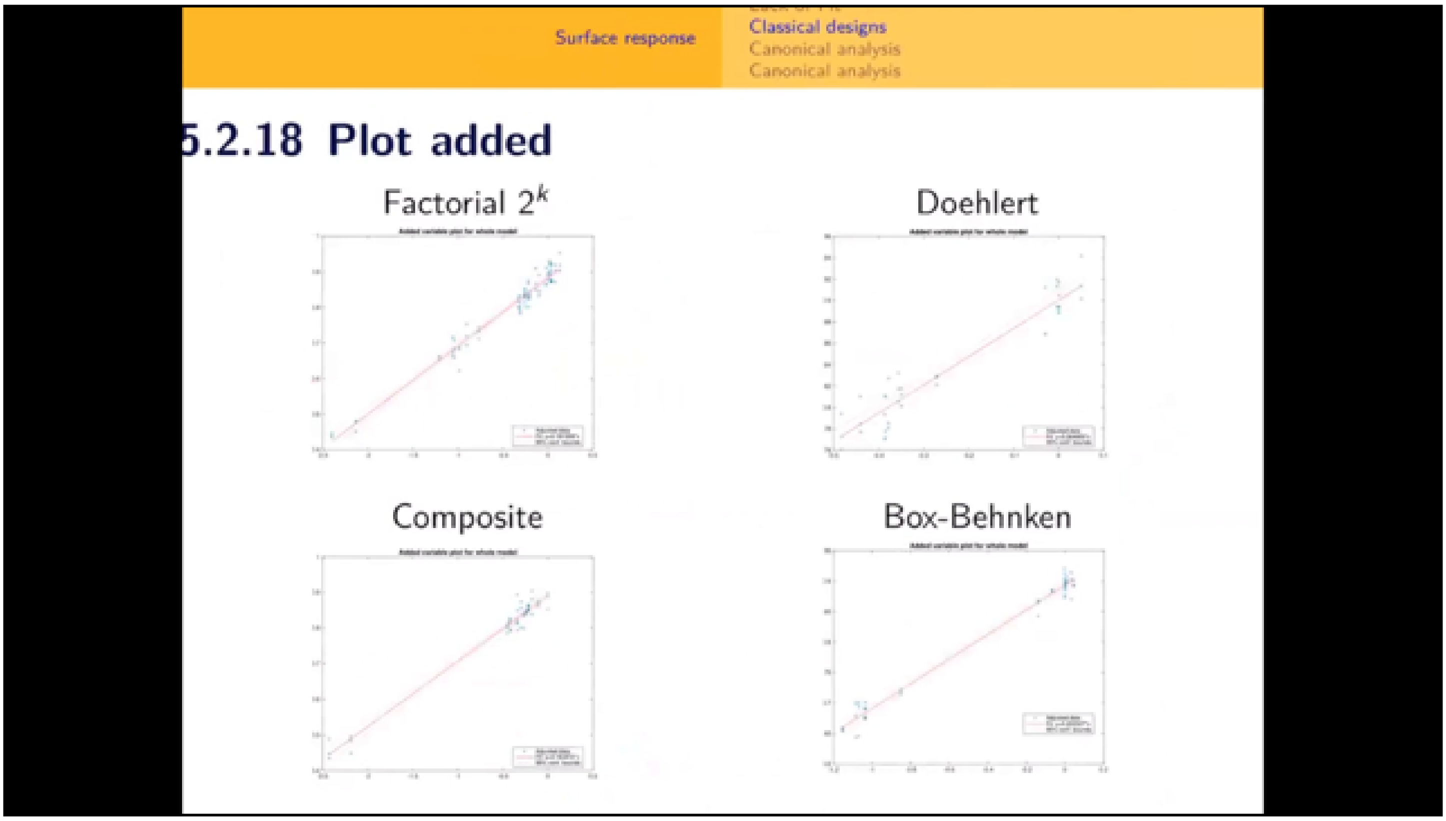
8m 59s



I also make a plot added. So it's why it was a possibility to check for the quality of my simulation from my movement with my model. It's why it's a comparison between them. And you see that my model have good P values. Nevertheless, you have points right outside of the 95% confidence.

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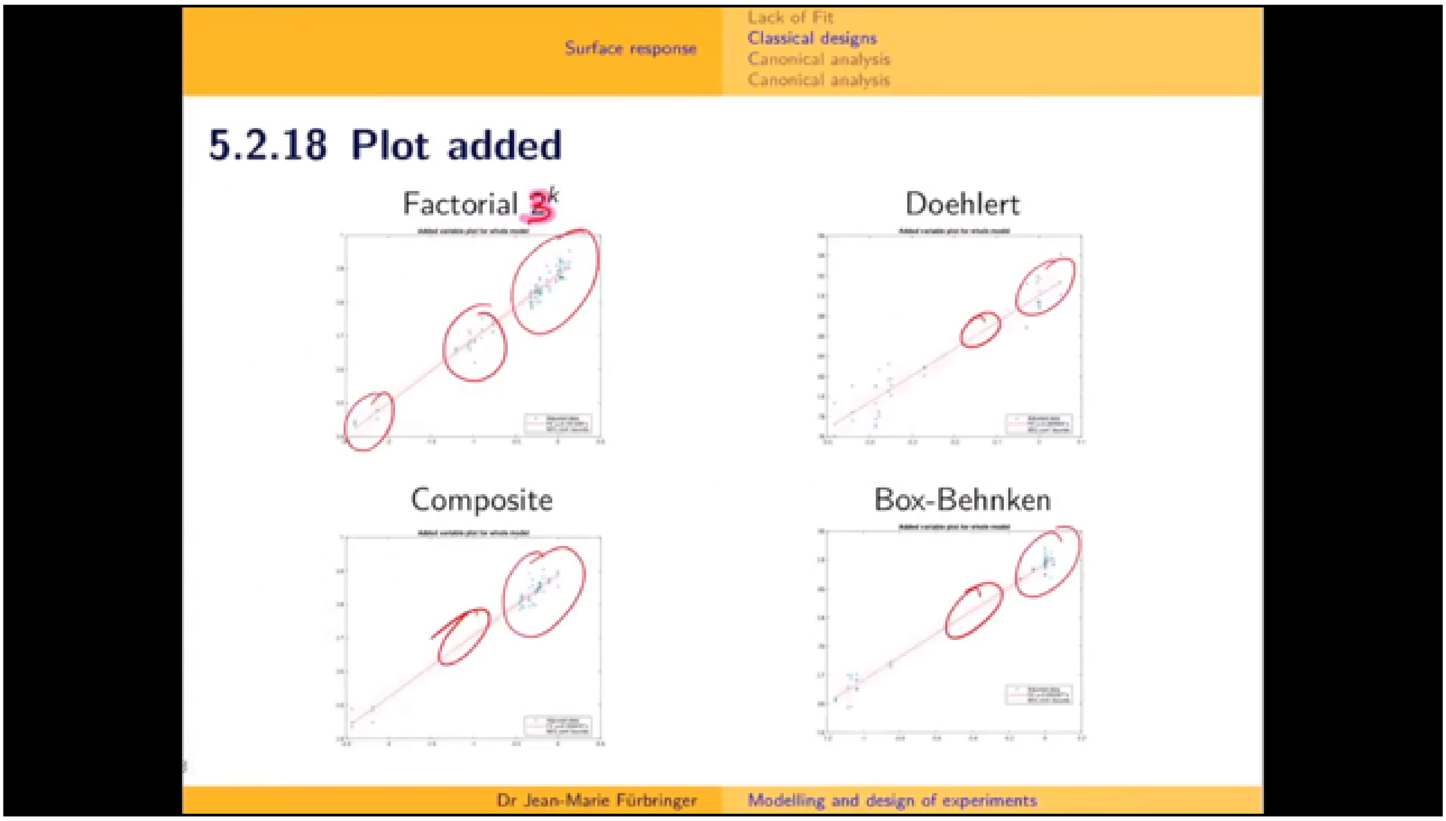
summary

9m 55s



And it's also perhaps explain a small difference. So you see the interest for the, oh, it's not two power K is three power three power K. And so you see that here you have some points at low value of your model. We have some points is the highest value of the model top of the of the of the heel. And we have a few points at the middle of the slope. When you when the other don't have this, this is a big difference between the three power K. The three power K have more points. Probably if you have a maximum as you have points distributed all over your domain, you have more points also at middle, middle value. Could be also perhaps a way of defending this design, which is expensive, but brings also a little bit more information than the other. But nevertheless, what I also observed that I have all the time a lot of discrepancies to my to my model. No explanation as my simulation as it was a simulation of a measurement. So for just random random error, but probably it could be interesting to understand understand that. So it would be quite a lot of variability. So this was for my explanation. So now I would like to introduce the last chapter, the last sub chapter in this chapter. It's called canonical analysis. So we have those function with coefficient of the second degree.

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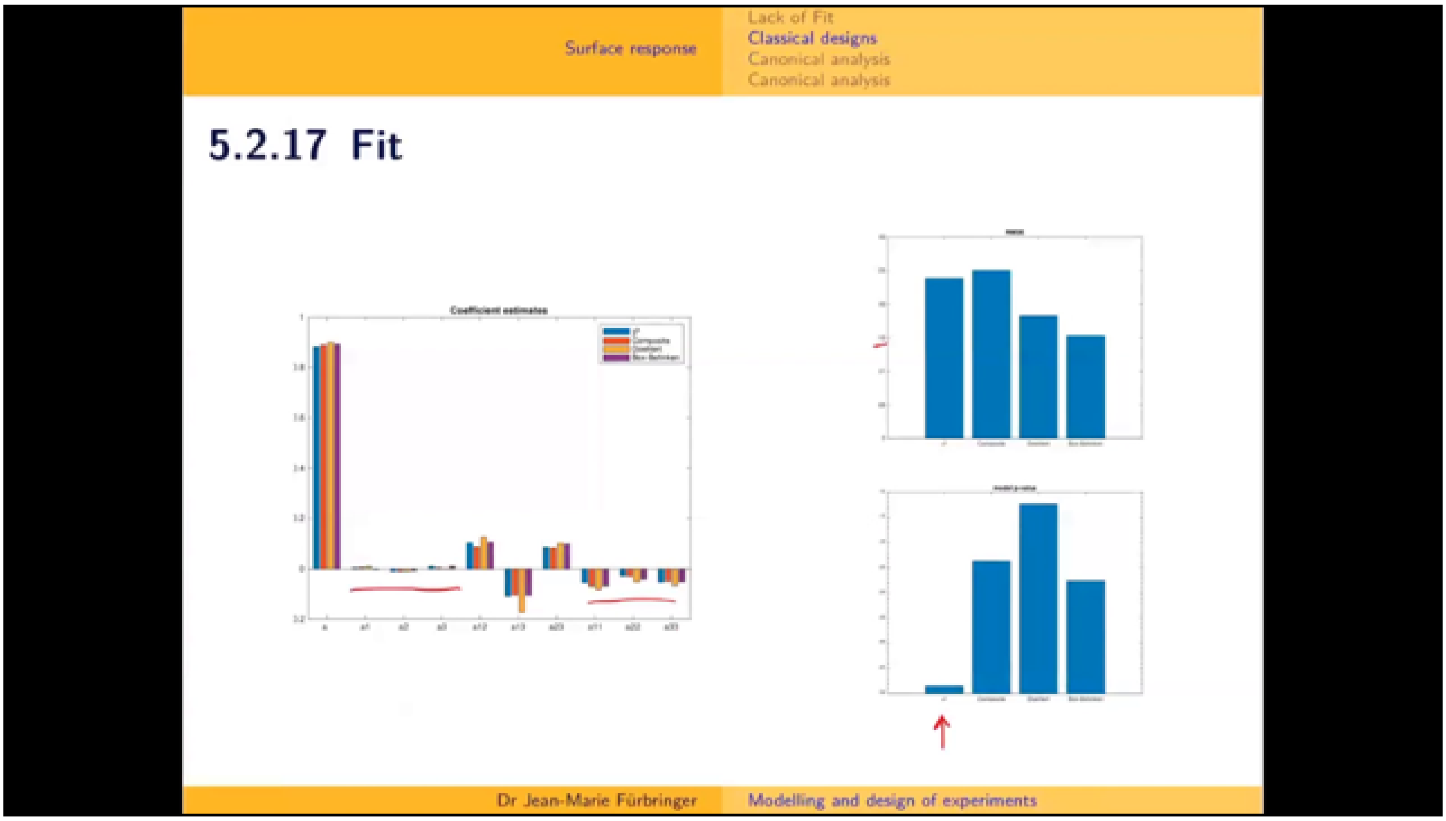
summary

10m 25s

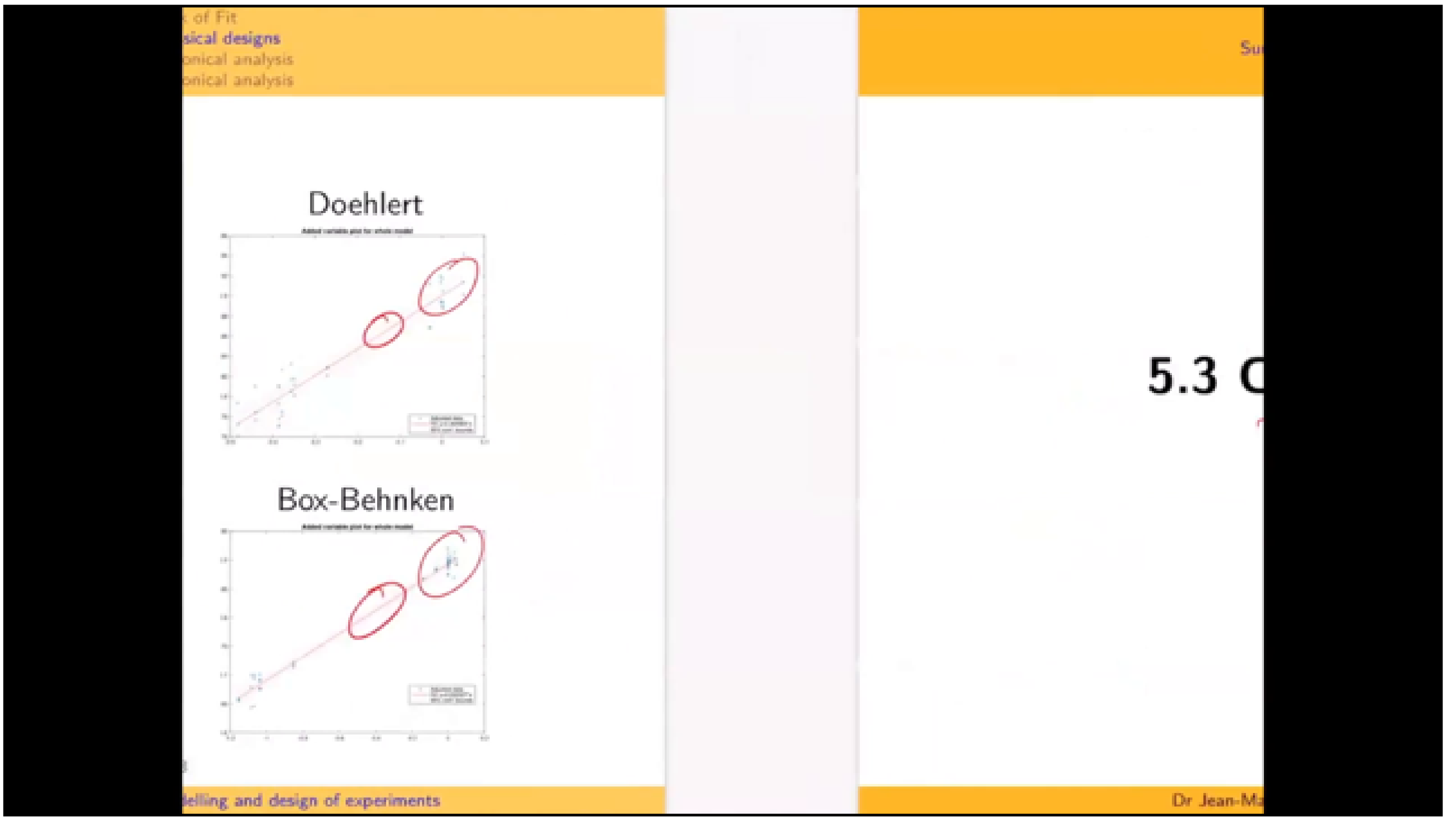


We can compare those values of the coefficient between them. But it's when you compare many effect, it's OK. It's it's you are saying, OK, these factors is more influence than this factor.

notes

summary

12m 20s



In the second degree, it's not exactly the same because you have courage. So it's you cannot make the same analysis. It's why our brain is so linear and we make some time big errors of estimation when we start having courage when we have interactions, things like that. So it's important to have a tool for understanding what's happened. So if you are with two factors, it's OK. You make a map of the values and you understand where you have heel when you have valley. You make a contour line and you can try to understand what's happened. If you have three, four, five factors, it's impossible to you can make math, but you have to make a lot of maps and you have to follow what's happened.

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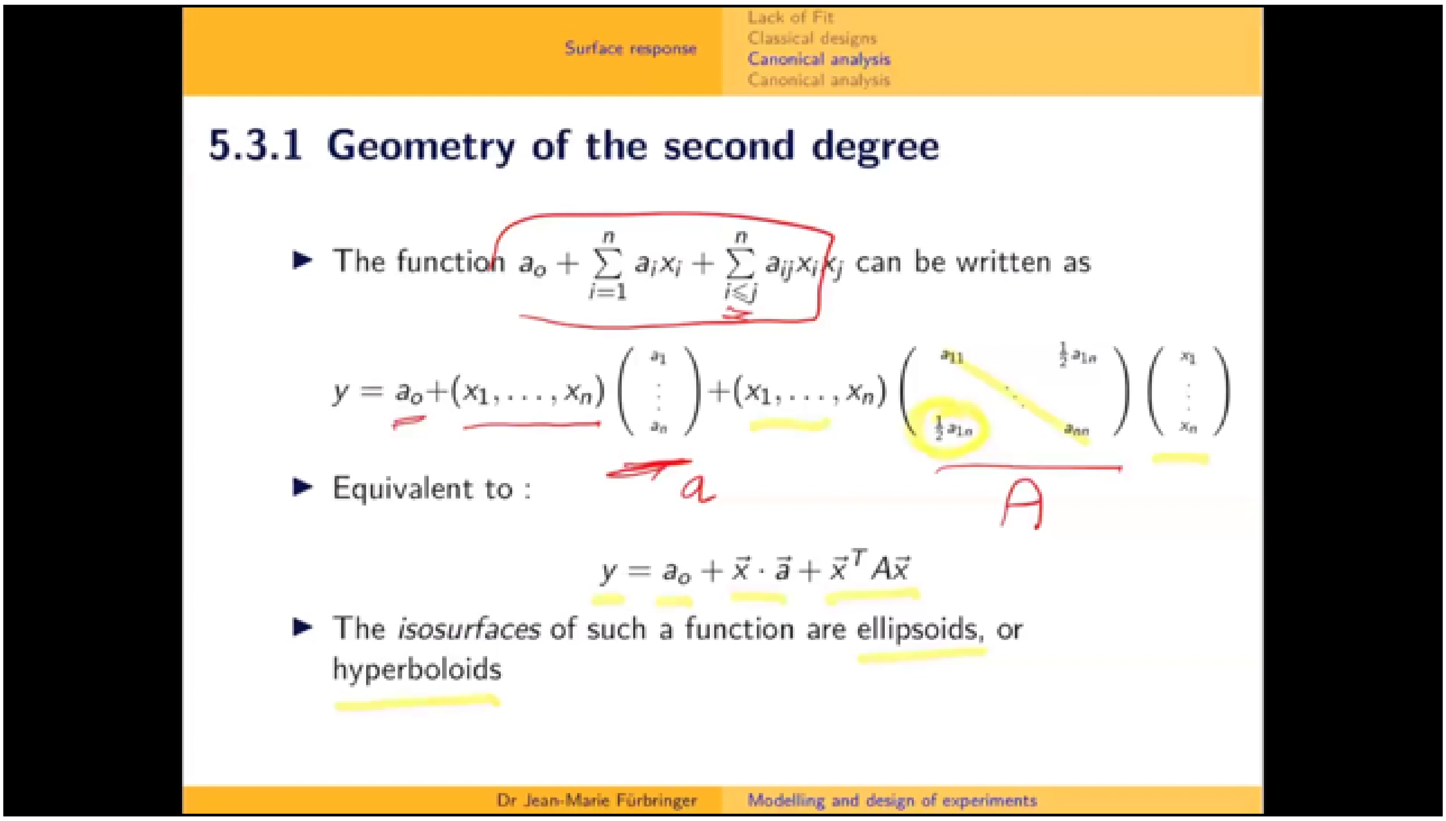
summary

12m 37s



So the canonical analysis is a way of getting insight in those functions. It's based on the second, the geometry of the second degree. So we start with the model of the second degree. Have we have we have it? Constant linear effect and the instruction and the second degree. We have a smaller equal to J. We can rewrite it differently. We can rewrite it geometrically. So if you have a course, usually it's in high school, no analytical geometry and things like that. When you play with plans with how the straight line is arriving, which which angles the straight line is arriving on the plane and all this type of problem. A lot of problems in the baccalaureate, a lot of problems on this. So you can represent your your function with a constant a zero with a vector of linear coefficients, which is multiplying the coordinates of your points. And with what we call the curvature matrix. So usually the vector of linear coefficients, I call it a and the matrix I call it capital A. And look, it's it's a little bit strange and it is built because you have on the diagonal, the quadratic terms. And you have outside of the diagonal half of the interaction. So you have such a matrix as soon as you have instructions, you can start making building this matrix A and making the canonical analysis. Before it's not interesting, you just have planes. So it's not interesting making a sophisticated analysis of planes. And so you have this matrix, which is multiply it's left and it's right by the coordinates because it's a quadratic terms. And it's because you have this double multiplication that you have half of the instruction outside of the diagonal because you have IG and GI, which are making the multiplication. So you have two times each instructions. So that's why you have half

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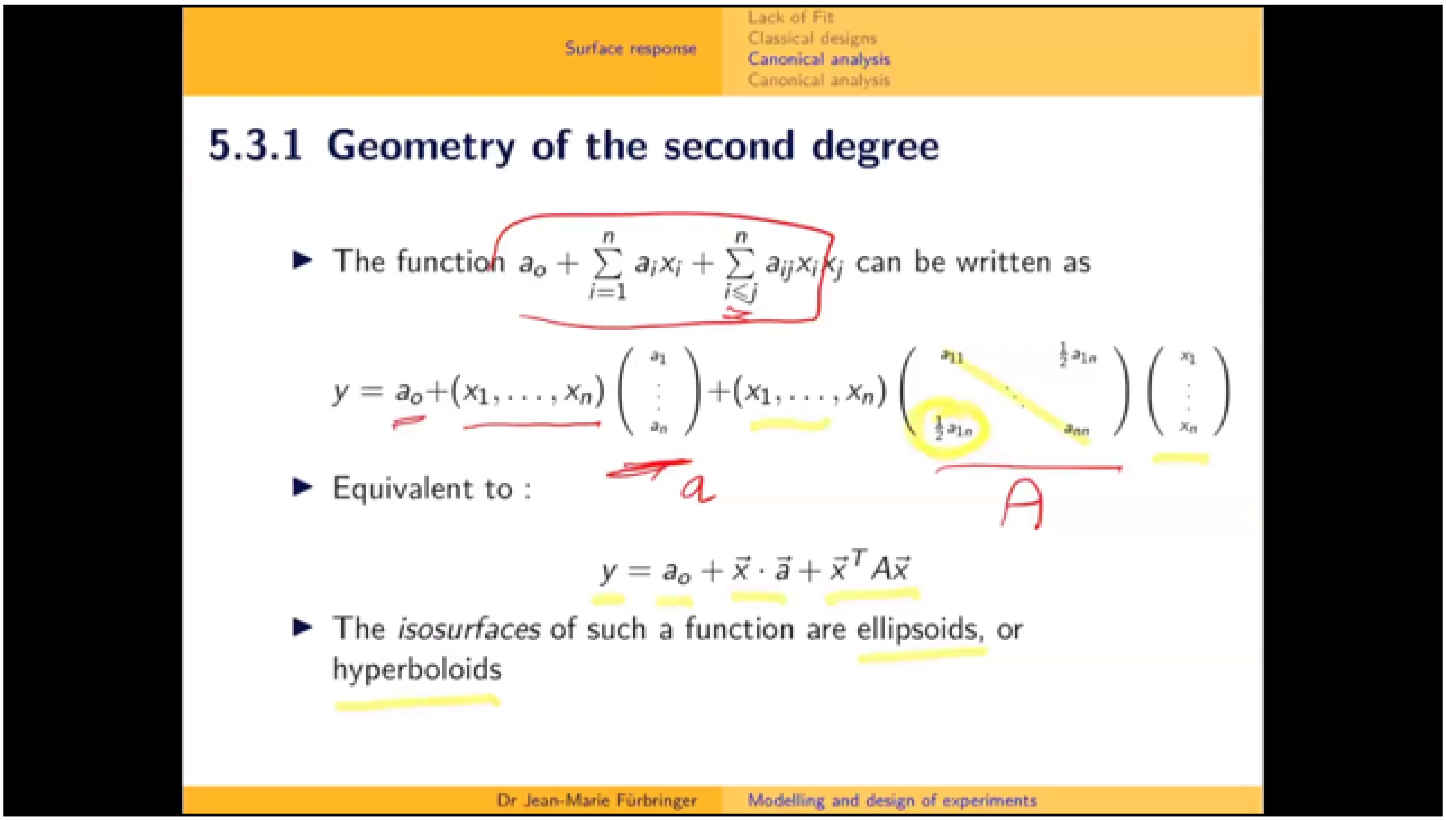
13m 23s



of it. So you can rewrite your function Y. As a number. As the multiplication of two vectors, one of the position one of the linear coefficient and matrix B linear. Relation with the matrix capital A, which is multiplied at side and left by the coordinates. And the geometry is fixed. You have two choice or you have ellipsoids or you have hyperboloids. So an ellipsoid is a root B ball.

notes

summary

5.4.1 Canonical analysis - fix point

- The center of the figure and the orientation of the axes, as weel as the ration of the axes is not knows a priori !
- The canonical analysis consist in determining those informations
- First identify the center of the figure that can be an extremum or a saddle point
- We look for a point defined by $\nabla y = 0$

$$
\begin{aligned}
\frac{\partial y}{\partial x_i} &= a_i + a_{1i}x_1 + \ldots + 2a_{ii}x_i + \ldots + a_{in}x_n = 0 \\
0 &= \vec{a} + 2A\vec{x} \\
\vec{x}_s &= -\frac{1}{2}A^{-1}\vec{a} \\
y_s &= a_o + \vec{x}_s \cdot \vec{a} + \vec{x}_s^T A \vec{x}_s
\end{aligned}
$$

So there's not exactly a root B ball, but understand that you have something. So typically you have a source of heat at the center of the body and you can see the heat map, the heat which is going outside of your body. Or the reverse. It could be a value, a property, which is increasing when you go out of one point or which is increasing or decreasing when you are going away of one point. But the slope of this increase or decrease could be not the same in different directions. And so the algebra tell us that we are only three factors. We have only three directions and we have some axes that are obligatorily at right angle. So it's obligatorily. It could be a root B ball. The root B ball have two axes that are the same. Three axes could be different in our students. So it could be a root B ball, but some directions that are different. And the hyperboloids. So it's the same, quite the same thing, but you have some direction where you have your property increasing and you have other direction when your property is decreasing. No other possibility with a second degree. The trick that the center of your. The center of the picture is not obligatorily the center of your domain. You can be in the pot. You can be just here, for example. But in any case, second degree, it's or an hyperboloid or an ellipsoid.

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16m 49s

5.4.2 Canonical analysis - main axes

- Main axes are the eigen vectors A, $\tilde{x}_1, \tilde{x}_2, \tilde{x}_3$
- The increase of the function $y = f(\vec{x})$ in the direction corresponding to the main axes is given by the eigen values, $\lambda_1, \lambda_2, \lambda_3$
- In the directions where the eigen values are bigger, the contour lines are close to each one
- The function y can be re-writen in a canonical form

$$y = y_s + \sum_{i=1}^{n} \lambda_i \tilde{X}_i^2$$

- If all the eigen values have the same sign the figure is an ellipsoid, in the opposite case the figure is an hyperboloid

Oh, the canonical analysis understanding if we have an hyperboloid or. Of an ellipsoid and understand what is its orientation and where is its center. So the first thing is easy is to check where is the center. So we find where the gradient is zero and the center is where the gradient is zero. So you can derivate the function and we obtain that the center of our figure is at the value minus one half of the inverse of the matrix of curvature. Capital a multiply by the vector of linear coefficient small a. This give you the position of the center fixed point we call it. And after the question is, is this fixed point within your domain or outside of your domain? Or if it's outside is close to your domain or is far away of your domain. So if it's far away, eventually you can forget the curvature and treat the problem with planes because you are very far away. If you are close to the center, you have to take into account of the curvature. And after you have obtained the center of the fixed point, you are interested to get the value at the center of the fixed point. And this is just applying the value XS or your fixed point to your model at that position. And you get the value X, Y, S, which will be interesting in a moment. After you would like to understand how are your figure is oriented. And for that, you have to calculate the eigenvalue and the eigenvector of your matrix a. So I didn't explain you how to do it.

notes

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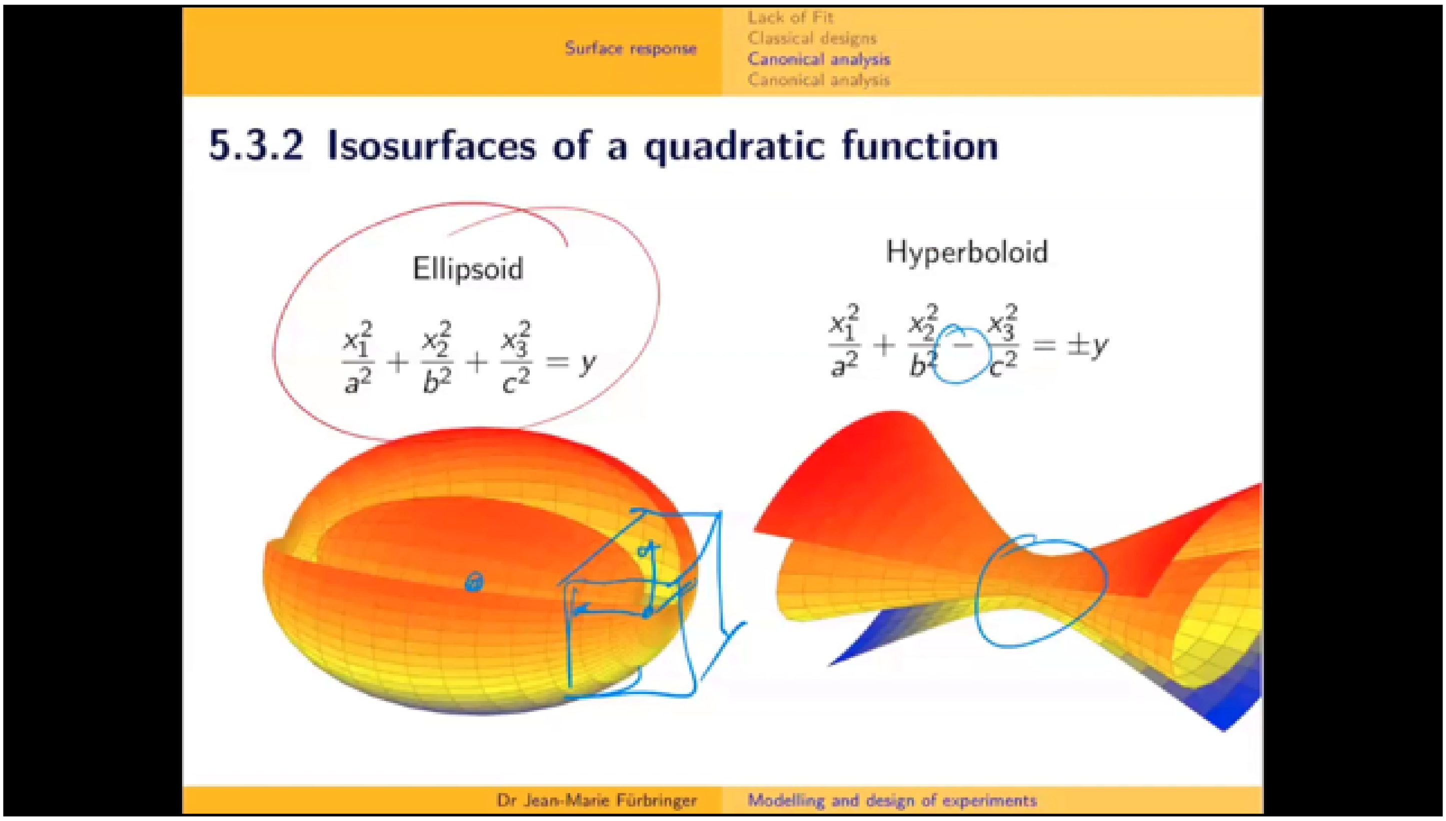
18m 51s



I consider that you already know it. Or if you don't know it, look at a book of linear algebra. How do you get the eigenvalue and the eigenvector? In any case, if you are working with Python, if you are working with Smart Lab, you have routines also that are giving you those values. So I will call the eigenvector a-kiss-tilde. So the linear algebra as my matrix of the coefficients, my matrix capital A is positive. I will have three eigenvectors that are not all positive, but that are what I wanted to say. They are orthogonal, one to the other. There are some properties. I'm not spending time on that, but there are properties coming from the linear algebra telling you that these axes are orthogonal. And at each of them, I have an eigenvalue. And this will tell me how many times I'm increasing the value of my property, when I'm modeling my y, when I'm following one eigenvector. So that means that if I have a high eigenvalue, that means I will increase rapidly. So my level curves, my contour lines will be close one to the other. And when I have a low eigenvalue, I will have a long axis. And then I can analyze that, so understand where I will show you in an example. I can show you where I have my center and around my center. I can draw those type of contour lines and understand inside of what I have in my model. It's easy to make it in two-dimension. When you have to make it in three-dimension, you can use iso-surface for representing the equivalent of the contour lines. When you are at four or more factors, it became complicated. So you have to look at the interactions and eventually separate your variable where you don't have instructions. You can analyze factors alone when they do not have interaction

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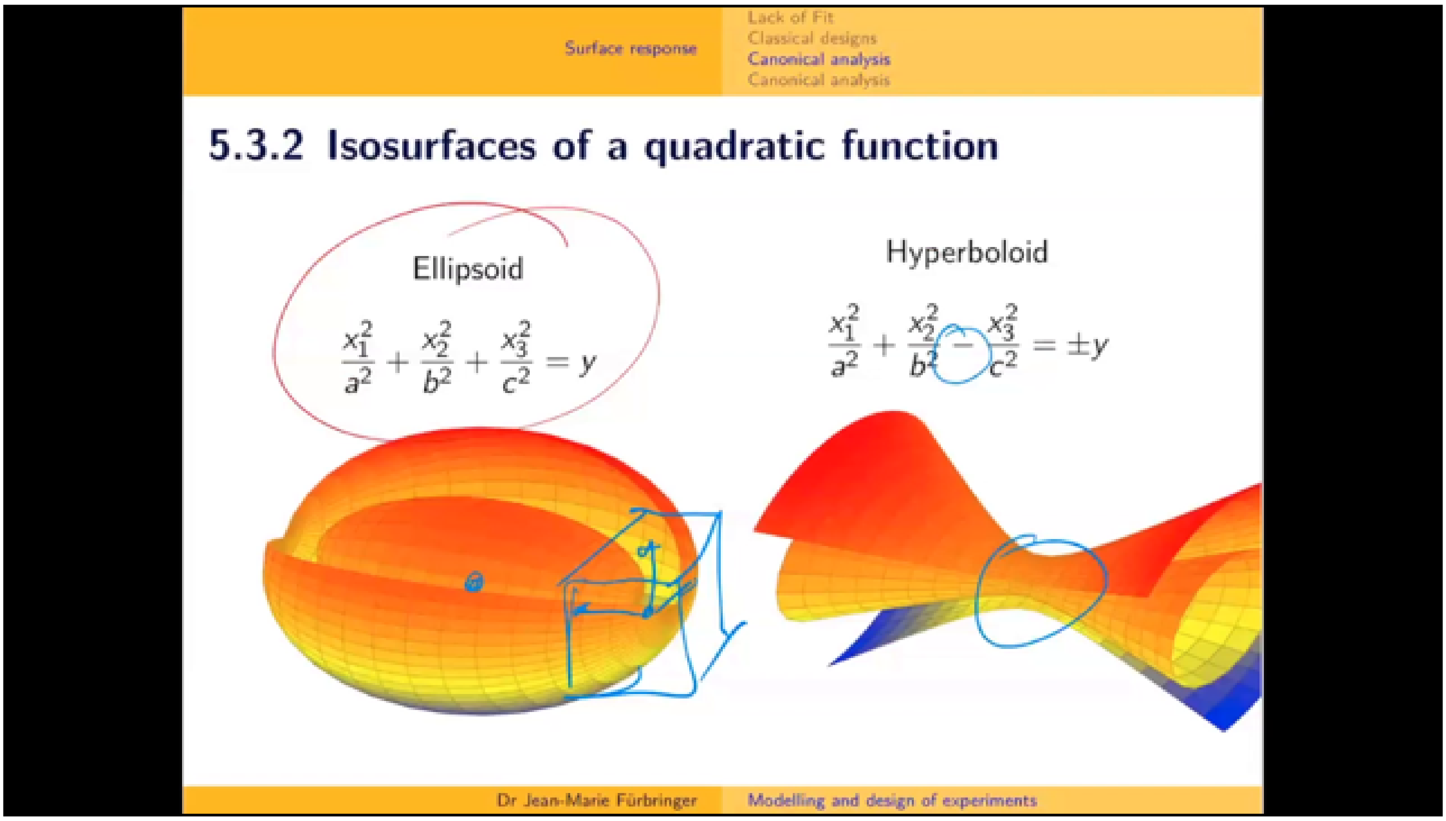

with the others. You try to make groups of variables where they do not have interaction between them or very small interaction between them and follow what's happened. It's not so complicated, but it's not so easy. And then you can make a new model within your following, your new axis. So you can change from your original axis to your new axis. That will be the eigenvectors. And in this eigenvector, so your function will have only quadratic terms. Because the interaction was because of the rotation of the eigenvectors in comparison to your original angle. And it was also the case of the linear coefficients that would depend on that. So now you can have what we call a canonical model, which will have the value as a constant, the value at the center. So you replace a0 by the value at the center. And after you have the sum of your eigenvalue multiplied by the coordinates in your new system represented by the eigenvectors. And you see that here the sign of the eigenvalue will make the difference. If you all have a positive or a negative, that means that you are in an ellipsoid.

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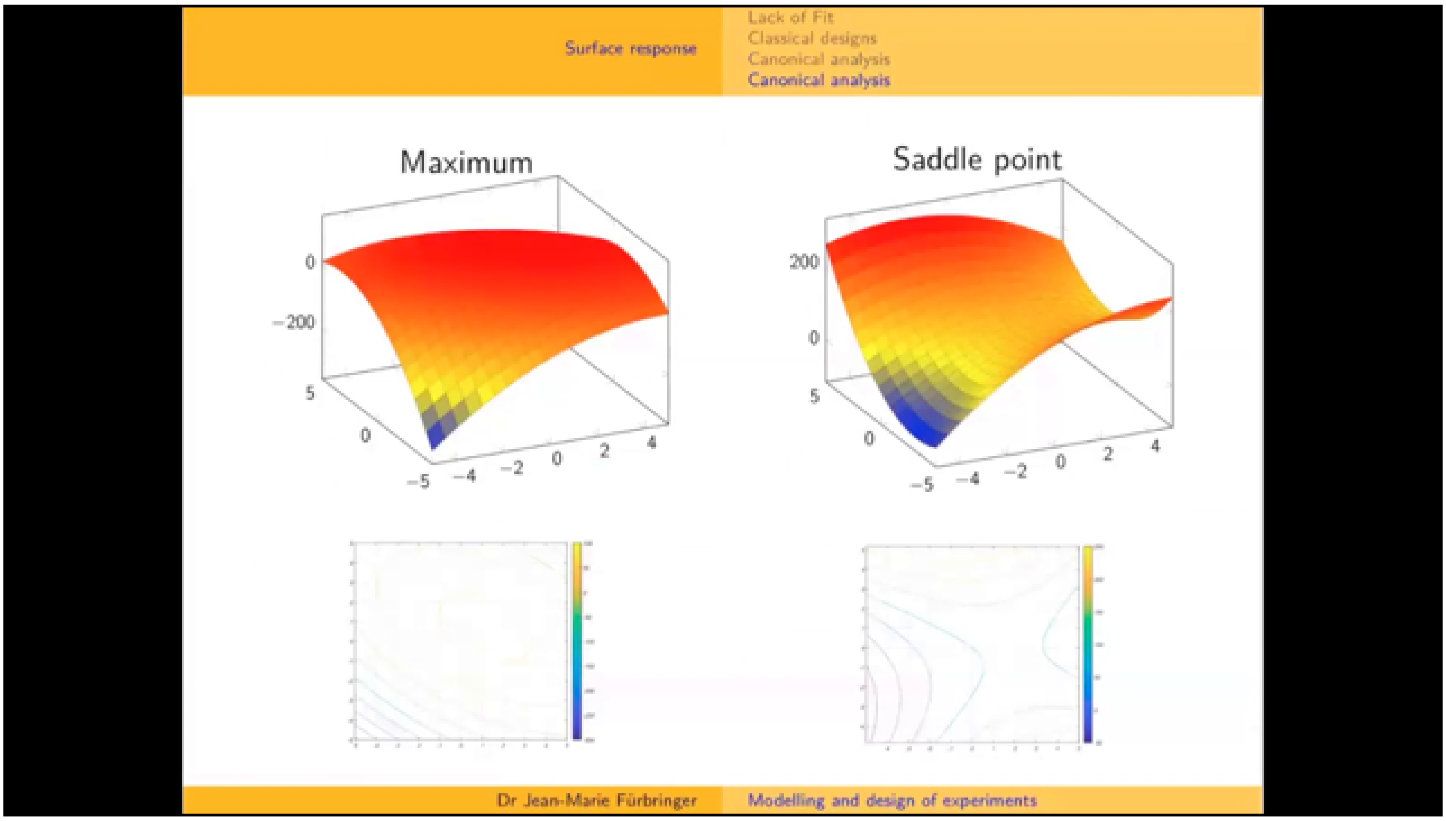

But if they do not have the same sign, that means that you have a hyperboloid. So for understanding what you have as a picture, you need to check the sign of your eigenvalue. All the same, root bb, different hyperboloid.

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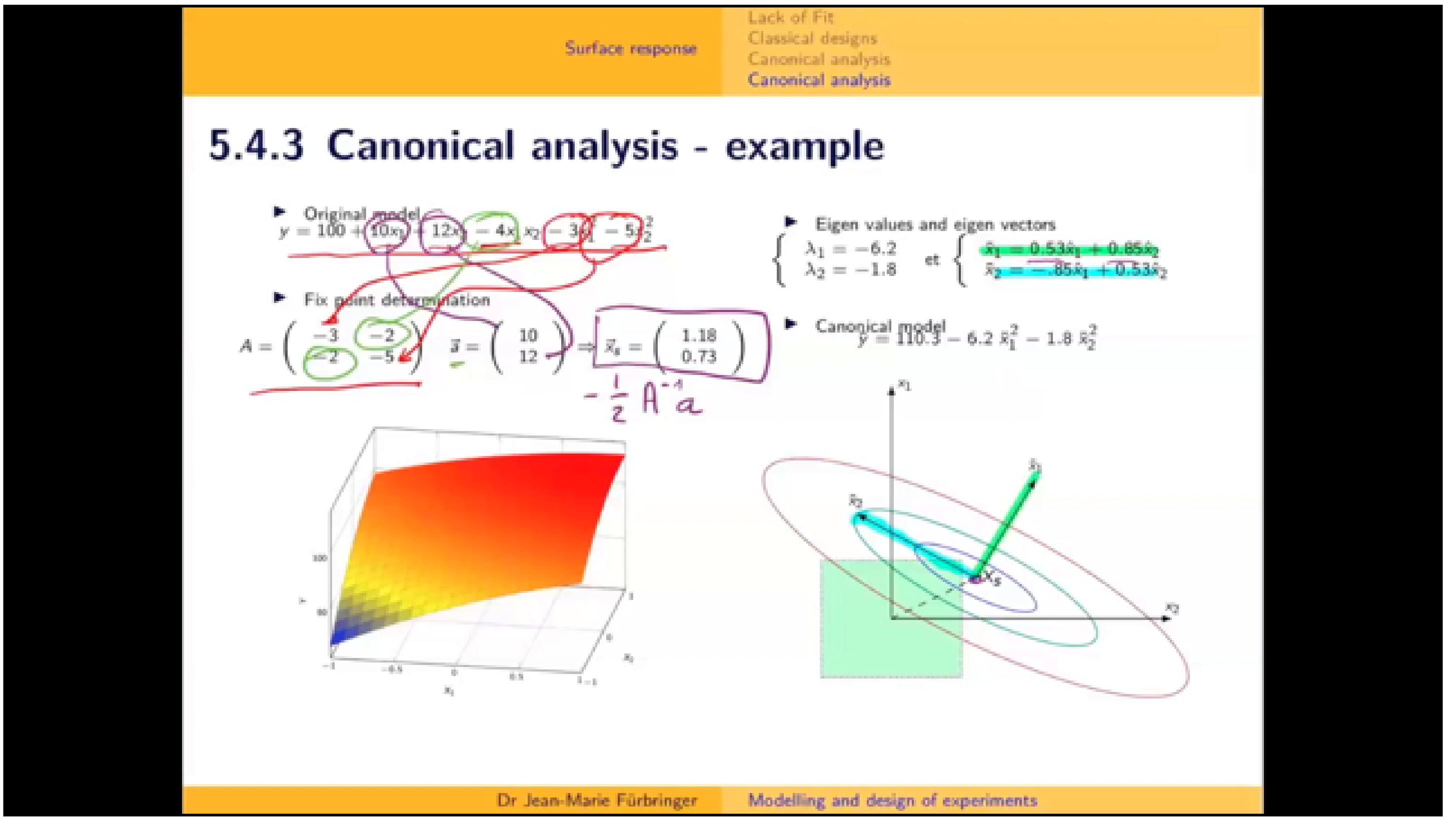
25m 13s



And then depending when you are, when you have a second degree, then you can be going up a hill. So it doesn't change a lot of things for your influence, except that you have a little of curvature. But it will change things importantly if you are at the top of your hill. And that means that you don't know if you see the contour line quite well. I don't see them so well in my screen, but you see them. So you see those lines. So if you are just in this place, you can treat the problem as linear. But if you are in all your domain, you better treat it considering the second degree with a maximum which theoretically should be right here. Or you are in a saddle point, you are in a pass, and it's quite interesting sometimes for a phenomenon because it's a very stable situation. And so in this situation, it's typically an hyperboloid situation. In some direction, you are going up and some other direction, you are going down. Here I make a small calculation of that. So imagine that after your analysis, you have fit a model, a quadratic model, was 100 as a constant, 10 and 12 as main effect, minus 4 as an interaction between x1 and x2, and minus 3 and minus 5 as a coefficient of the second degree. So I built the matrix A. So minus 3 here is now here, minus 5 here is now here, and I have an interaction of minus 4, which is became minus 2, and minus half of the interaction coefficients. My vector A will be 10 and 12, and then with that calculating minus 1, half A minus 1A, you are able to calculate the position where is my center. And my center is in 1.18 and 0.73. So I'm outside of my domain, but quite close of

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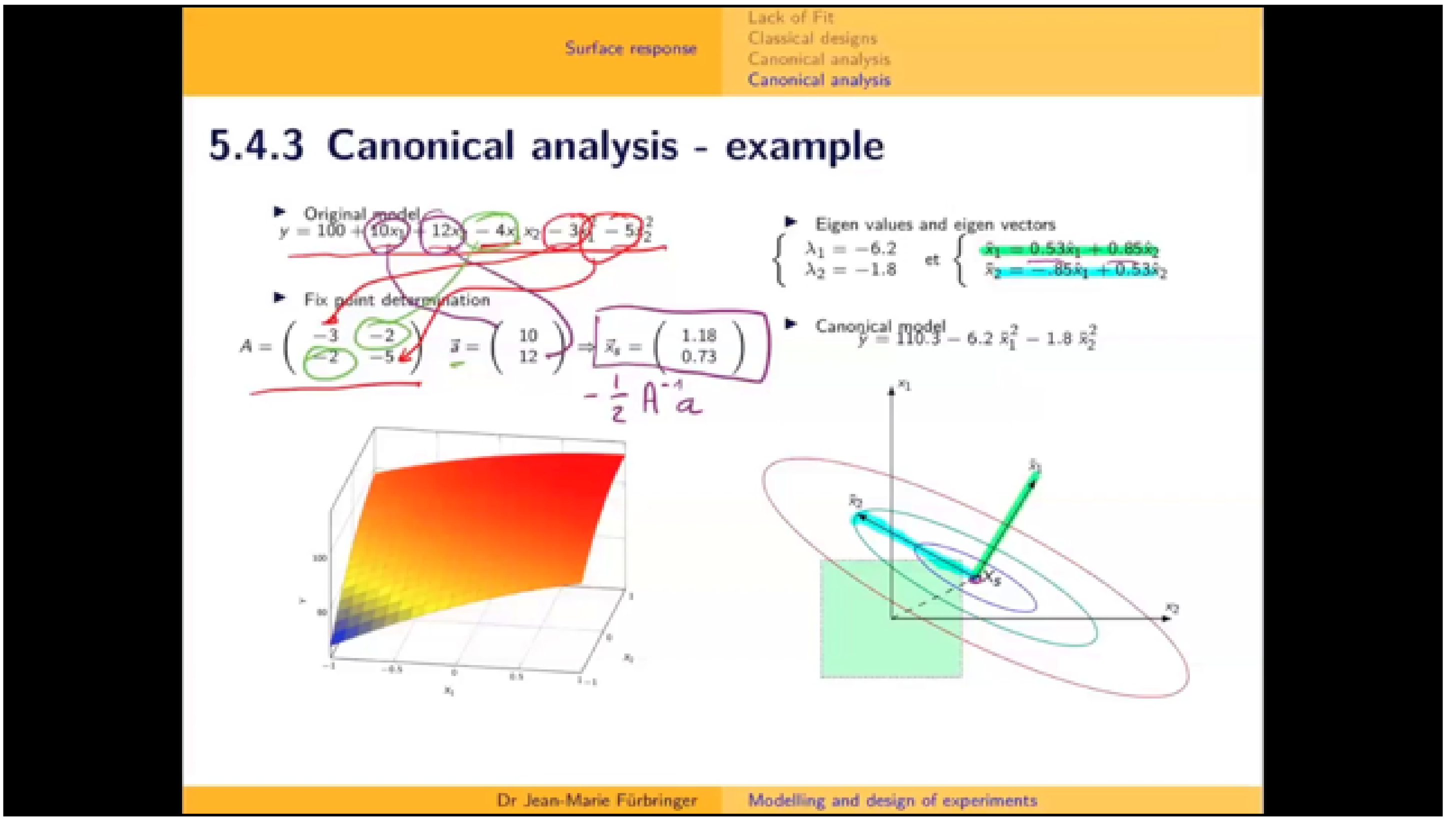
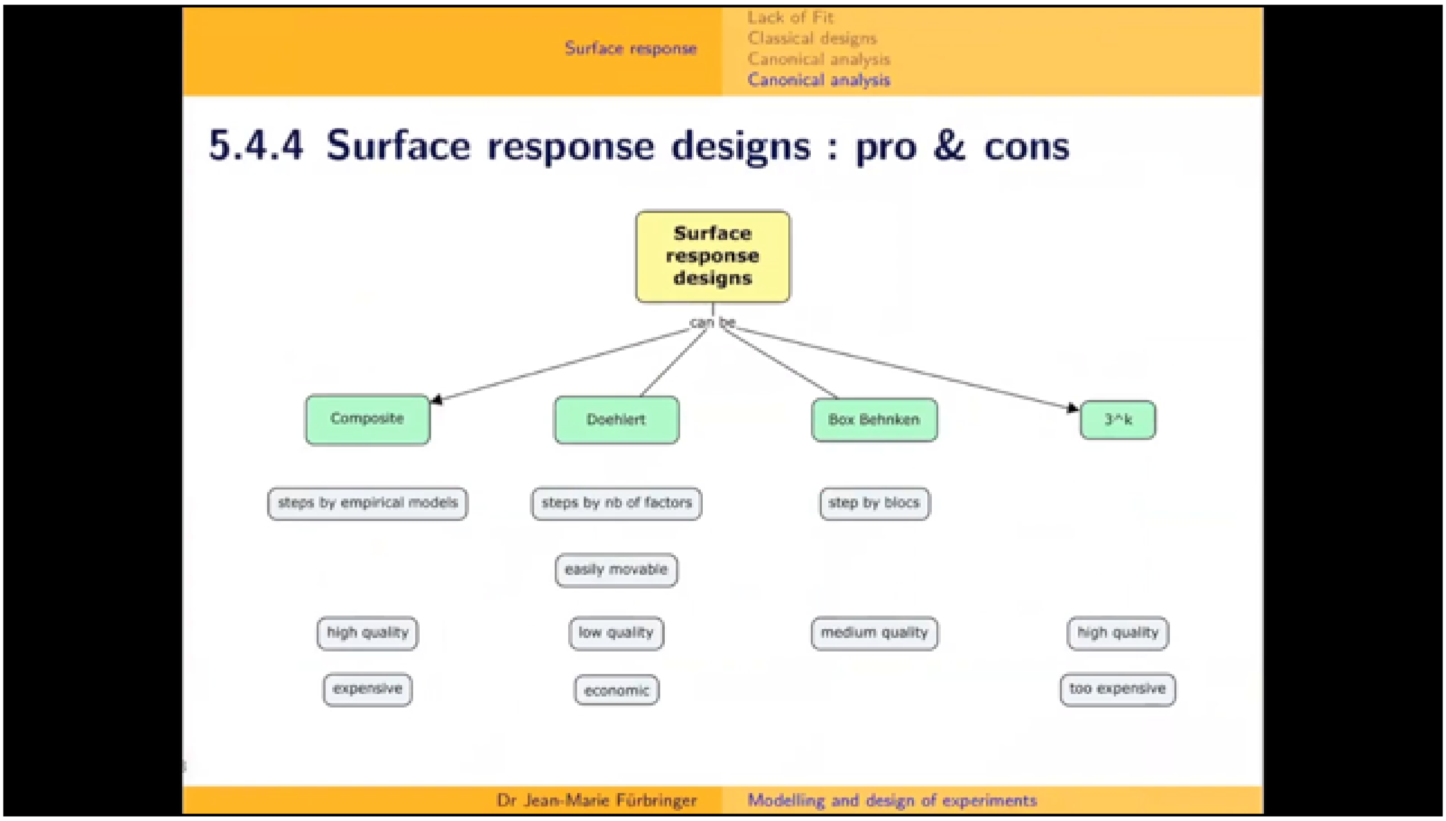


my domain. So my center is if in green you have your domain, my center, my position of excess is here. After I calculate the eigenvector, and I'm calculating my eigenvalues. So my eigenvectors give me 1, which is 1.5 x1 and 1.80% of x2, so plus plus. So it makes this, it makes this axis. So this is makes this axis. And the other is perpendicular. So you change the coordinates and one have to became negative because you have a rotation of 90 degrees. And then you have, I'll take another color, I take blue. So this one became this axis. And now I look at the eigenvalue. So I have two eigenvalues that are negative.

notes

summary

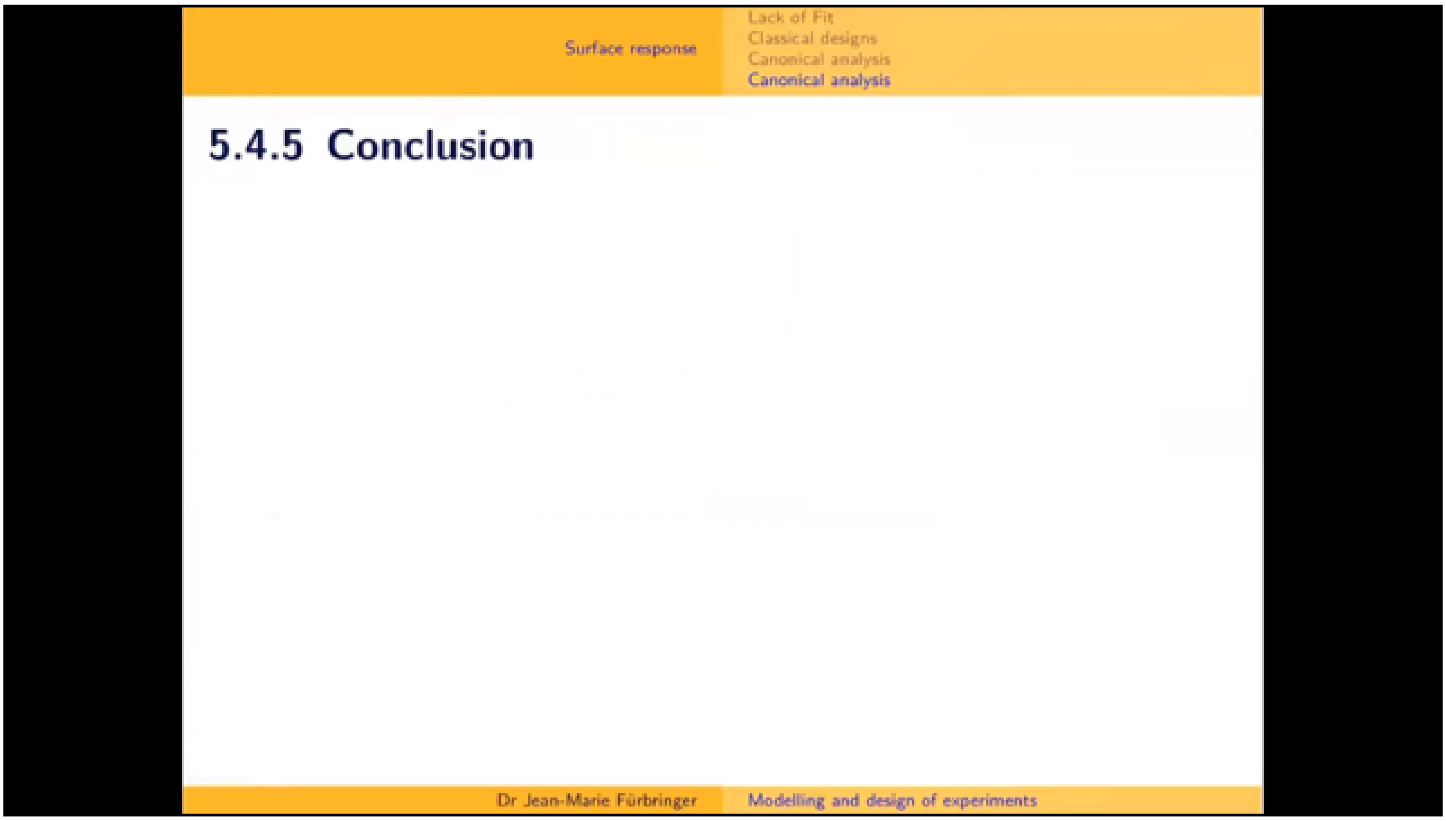


The eigenvalue related to the first eigenvector is six, minus six. The other is minus two. So one is three times bigger than the other. So if I have here the eigenvalue lambda one equal minus six. So it's where I have my contour lines closer. And in the other, they are quite three times smaller than the eigenvalue. So here lambda two equal minus two just for simplifying. So that means that I have no lines, contour lines that are three times larger. And now I'm able to draw my contour lines. It's an ellipse because it was all negative. And so I have my function. It's represent a situation where I have a center, which is a maximum outside of my domain. And after I'm decreasing my value. And so if I'm looking for the maximum, my maximum is probably somewhere here. If I'm losing for the minimum, the minimum is probably here. So now you have seen a few designs. Eventually you arrive to second degree without those beautiful designs you do as you can with your data and etc. But you are able to understand. So it's true dimension is not the most practical. The chemical analysis because you can just make a map of your domain and you understand where you have your maximum, where your minimum. This became very interesting when you are in three and more dimension. So in the exercise, you will see and I show exercise where you can play with three and four dimensions. And observe when you do that to sometime have to have tricks to see if you are one variable, which is who to have no second degree or one variable that have no interaction with the other and make groups of three. If you can make group of three, you can understand something. If you cannot, it's became quite complicated to see what's happened.

notes

summary

29m 25s



Okay, so I show you three typical, four typical designs. They have different properties, different price, different accuracy. This map is summarizing a little bit what we have seen today. And with this, I'm finished with those classical designs that we find in response surface. As I mentioned, it's nice to be close to those designs because we understand it's what work. After we do what we can, very probably you have a plan and you do not realize exactly your plan. And after you have to check the quality of your design, you can improve, you can, you still have the tools that we have for the first degree, for diminishing the numbers of experiments, checking what is the value for the dispersion matrix and the variance inflation factor, for optimizing and having the good tradeoff between the numbers of experiments, the quality of your data. In that aspect, there are no difference between the first degree and the second degree. Remember, you cannot have orthogonal design for the second degree. They are all the time an alliance between the second degree coefficient and something else. If it's balanced design, it's with a constant, but it's not the balanced design. It could be with something else. Try to diminish them, but you cannot totally avoid them. And that's it for this chapter. You have some designs, train them, you have some routines for having them. And as all the time, planning is good. We never realize exactly what we have planned. So it's nice to be agile for adapting to the fact that eventually the design you realize is not exactly the design that you play.

notes

summary

31m 45s