



Course material

Course:

ENG606 / PHYS 442

Video:

DOE_lesson13_part2_CCM-mixture

Concepts (extracted from automatically generated subtitles):

Least having pairs. Classification of the different situations. Split plot. Presentation of things. Much test. Different sets. Greco-latin square. First level of statistics. Different animals. First thing. Lot of variability. Different place. Quite very interesting way. Least things. Triangle plots.



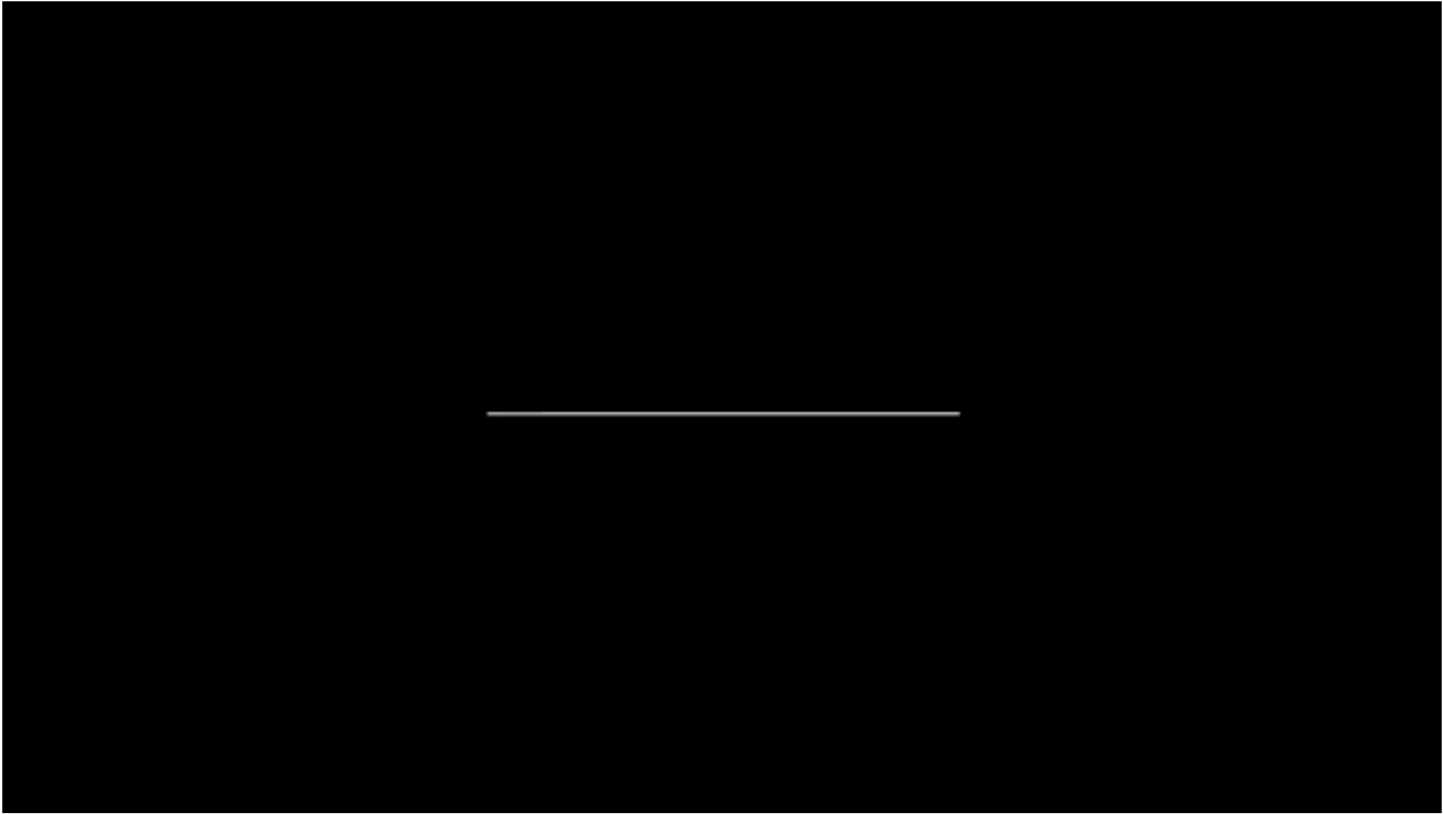
[to video sequence search](#)
(within ENG606 / PHYS 442.)



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summary

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6.34 Youden squares

A Youden square is a type of Latin square where each row and each column contains a unique set of treatments or conditions.

| | B_1 | B_2 | B_3 | B_4 |
|-------|-------|-------|-------|-------|
| C_1 | A_1 | A_2 | A_3 | A_4 |
| C_2 | A_2 | A_3 | A_4 | A_1 |
| C_3 | A_3 | A_4 | A_1 | A_2 |

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These subtitles have been generated automatically So, a Uden square. So sometimes you do not have sufficient levels in your variables.

notes

summary

0m 1s



6.34 Balanced Designs in DOE

- ▶ **Completely Randomized Design (CRD) :**
 - ▶ Each treatment is assigned to experimental units completely at random.
 - ▶ Ensures that every treatment has the same chance of being applied to any unit.
- ▶ **Randomized Block Design (RBD) :**
 - ▶ Experimental units are divided into blocks based on a known source of variability.
 - ▶ Treatments are randomly assigned within each block, balancing the design across blocks.
- ▶ **Latin Square Design :**
 - ▶ Controls for two sources of variability.
 - ▶ Treatments appear exactly once in each row and each column of a $k \times k$ square matrix.
- ▶ **Graeco-Latin Square Design :**
 - ▶ An extension of the Latin square design that controls for three sources of variability.
 - ▶ Uses two Latin squares overlaid so that each treatment combination appears once.

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So the Latin square and Greco-Latin square are working when you have the same number of levels per for each factor. Three for each one, four for each one, five for each one, etc. When you do not have it, you could have one with three, one with four, etc. So you have some tricks. So the Uden square are a sort of Latin square where you have cuts, one line. So there are a few designs like that. So you have here an example and usually, let's say for scientists, physicists is not so complicated to understand. The fight is between statisticians to calculate exactly those probabilities. So I hope I'm not making a picture too negative of statistics because I like statistics, but they are first level of statistics, let's say every day or standard experiment statistics, which is quite nice. And after you have some discussions deep on the really accuracy of the probability, etc. Usually in science, we say that don't spend more time determining the error than you are spending time for determining the effect in itself. So, yeah, sometimes I'm taking some shortcuts. So going back to the Uden square, when you have a situation here, when you have A and B that have four levels and you have C that have only three levels, and this is a possibility to organize your experiments and after. So it works the same, the algorithm, Anovan will work very well after it could have a few details on the calculation of some probability that could be. This is one of the solutions for treating if you have not all the same level. After it's a presentation of things that exist in the classification of the different situations, depending what you have. So if you are rich and you can make all factorial design is very good, but it could be expensive, etc. So this are some

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0m 5s



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cheaper situation. So the first thing is if you cannot do everything you want, the first thing is to have random choice of what you are doing. So it's all the time the first things to do if you have different sets to choose things at random, to make experiment at random, just to be sure that you do not have aliases between your experimental situations and your factor. So what we call completely randomized design, you have treatments that are assigned to experimental units. So treatment, you understand you're doing, you are doing something, it's come from biology and chemistry, typically this type of of wording, and your experimental unit is what you are testing, all the different animals, the different place, etc. that you are analyzing. So each treatment is assigned to experimental unit completely at random. So it's clear that if you have to make

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6.34 Balanced Designs in DOE

- ▶ **Youden Square Design :**
 - ▶ Derived from a Latin square, but with one fewer column ($k \times (k - 1)$).
 - ▶ Useful when there is an unbalanced number of treatments or when one treatment is repeated.
- ▶ **Factorial Design :**
 - ▶ All possible combinations of levels of factors are investigated.
 - ▶ Can be balanced by ensuring equal replication of each treatment combination.
- ▶ **Balanced Incomplete Block Design (BIBD) :**
 - ▶ Not all treatments are applied in every block, but each pair of treatments appears together in the same block an equal number of times.
 - ▶ Balances the design even with an incomplete representation of treatments.

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some treatment and you have different treatments that you want to put together, if you do everything at random, at least you protect of the fact that you have treat only a part that you already shouldn't, you take all the black guinea pigs for making one test and all the white guinea pigs for making another test, it's not a good idea. So you understand that. So this is the level zero of good practice. After you can have blocks, that means you make things by different operators, you have different havens for preparing your things, different laboratories, you have blocks, we already talked about blocks. So you show that random the different units in the different blocks, you don't choose again, you don't give the black guinea pig to one group and the white guinea pig to another group. After you have the Latin square, so this is a quite very interesting way of making not the factorial design, not all design, that it's implication that you need to have the same numbers of level and it doesn't, depending on the numbers of factors that you would like to test, you don't have everything you want, but even if you can do that. So you see, I'm going up the steps with situations that are each time more sophisticated. And so Latin

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3m 49s



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square, Graeco-Latin square design is with more possibility. The Uden square, so it's give you, it exists a few squares and when you don't have the same number. So some situation of solutions, some other nots. After the factorial design is the best in the situation because you test every possible combination between your factors and as let's say the most comprehensive. And after, let's say we go down again the stairs, something is called balanced incomplete block design. You have not all treatments that apply to every blocks and you start to at least having pairs. So this is what we check with the Latin square. If you cannot have all triplets or all quadruplets, at least you can try to have all pairs at least things like that. So it's what is called balance incomplete design. So what I'm expecting from you is that you exist, you know it exists. I'm not pretending that just having two slides on this, you have understand everything on this, but at least you know that it doesn't exist only Latin square and factorial design. It exists other way of treating those qualitative factors and that the basics at least is to use random choice just to be, yeah the random choice for just to be sure that you do not have bias. So random choice. Now if I depend random of what? So random of the order, but this I was making the random of the combination between two factors, typically if you think machines and tools and material and pieces. So if you cannot do all, you cannot do all the factorial. First you try to do the factor if you

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5m 27s



6.34 Balanced Designs in DOE

- ▶ **Split-Plot Design :**
 - ▶ Two levels of randomization : main plots receive treatments, and subplots within main plots receive
 - ▶ Ensures balance within the main and subplot treatments
- ▶ **Crossover Design :**
 - ▶ Subjects receive multiple treatments in a sequential order
 - ▶ Balanced by ensuring each treatment is applied in each position across different subjects.

have time and money etc. If you want to economize the time you can try to make Latin square, if you cannot at least, let's say that at least make a completely random design. And if you want to test that but you have to test that in two to two plans of your company try to make which would be a block try to use that. So there are three, three tricks, tricks is a little bit negative but there are ways of avoiding bias. You got me?

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7m 49s



6.34 Balanced Designs in DOE

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 - ▶ Balanced by ensuring each treatment is applied in every possible position across different subjects.

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There are still two things again I just put them because I would like you know it exists but if you are interested you have to dig. I'm not all come back perhaps next year, perhaps next year I will dig more in this. I'm not sure it's in this course is really interesting to dig more because the probabilities that you will have those situations is quite low but I just wanted you to know that they exist. So something is the split plot is the answer when you have different level of variability with your factors.

Typically the split plot is very, so split plot is coming from your garden so you are testing things in different plots of your garden that eventually are not the same because you are putting some products, some cements, some different things but the plots are very different in your garden. One is more in the south, one is more in the north, one have more sand, one have more I don't know another soil etc. So it's where it comes split plot. So the idea is not testing your different spinach, species of spinach one in one plot and one in the other plot because if the two plots are different you better have split your plot to be sure that you test your spinach at the sun, at the plot which is at the sun and you are also testing the two types of spinach in the other. You get again the idea. So it's called split plot and they are different way of analyzing the error when you have a lot of variability. So I don't think you will cultivate spinach so much during your PhD. What could be interesting when you are making tests with people because the variability between people could be very different. So if you are and sometimes you cannot test people with so many

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8m 28s



6.34 Balanced Designs in DOE

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different tests so you have to choose. So this is when the split plot could be of importance. I know there are a lot of research here for medicine, for device, medical devices etc. and many times in medical devices you cannot make too much test with one person and another person is different. So this is where split plot. So just it exists and if interested it exists books and probably a lot of books on split plot this is a very interesting concept and the crossover sorry I don't remember if to read it. It's quite the same thing but so split plot probably is between one treatment and when we have several treatments there are a way of balancing the different treatments that you apply to different. So statistic is quite a huge field. There are a lot of things. It exists more than

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6.35 Conclusions



what I'm trying to teach in this course or perhaps the meaning of those slides. It exists other things so go digging in this direction if you need if you are interested. The crossover I don't know it so well. Split plot could be one of the interesting things.

notes

summary

11m 37s



Modelling and design of experiments

Chapitre 7: Mixture designs

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Fall 2024

We have worked on constant coefficient model and also random coefficient model. They are very common in biology in medicine. There are less comments in engineering but more and more you could be able to differentiate between different strategy of production different recipes so it could be interesting to know those models. There are probably the statistics is a little bit a little heavier than in the parametric model. We are more used in the course of physics. We are more used of this parametric model. There are of importance and remember they exist and use them what it's useful. There are a sort of statue and I mentioned that so you see the muscle but it doesn't work. So you can learn a lot of things but you still usually when we are modeling something when we sing in engineering making a model of something we sing something more complicated that those type of model. But when the situation we are today close to production also if I imagine all this type of scenario for climatic problems etc those type of model could be quite very good. Strangely with the year each time this chapter for me is taking more importance. Now I would like to start the next chapter.

notes

summary

11m 55s



7.1.1 Specificity of mixture spaces

- ▶ A mixture space is considered when the factors x_i are fractions of a whole and that the increase of one factor implies the decrease in proportion of one or more other factors.
- ▶ This situation then implies in addition to the model $f(\vec{x})$ to be determined, two other conditions :

1. a constant sum : $\sum_{i=1}^q x_i = 1$

2. positive values $x_i \geq 0$

So now we are changing completely the situation. We are coming back to parametric model but we are trying to make a design of experiment for situation when we have a recipe. The particularity of recipe is that we are talking in fractions of products. So it's Christmas so perhaps you are making cookies. Cookies are making all the time with flour, eggs, sugar. So you understand we are working with in this situation with recipe. In engineering there are a lot of recipes. There are a lot of situations in which we need to have 100% of something and we have to manage the percentage of each one. So it's what we call mixture design. In chemistry is the art of chemistry. In physics it's happen. It's not so common but if you are preparing materials typically you have recipes etc. So there are a few rules this condition. So when we have a mixture that means we have one additional equation for all the models we are. The fact that we are working with concentrations, the sum of the concentrations must be one. So it's an additional equation in comparison. So it's diminishing the rank, the degrees of freedom that we have. So it gives us several possibilities. There are a few situations in which mixture can be treated exactly as we have done with factorial design, with plaquette and brumane design etc. But there are other situations where we can take profit of this additional equation. It's what I want to present in this chapter.

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13m 34s

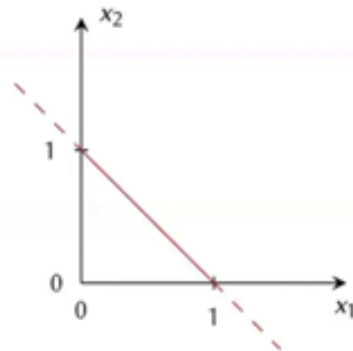


7.1.2 A mixture of two components

- ▶ Simple example to illustrate the principle
- ▶ Two variables x_1 and x_2 like the concentrations of two products :

$$x_1 + x_2 = 1$$

- ▶ The experimental space has one degree of freedom only



We have another also particularity of this situation that we will not work with normalized variable because we don't understand what would be a negative quantity of sugar if you would appreciate it perhaps. But so we ask all the time with positive quantities and we are not normalizing the data between minus one and plus one. We could but it's it became a nonsense and after we don't understand what we are doing. So we prefer stay in a situation where we have values that are smaller than one, one being 100% and bigger than zero. We are working with ratios of

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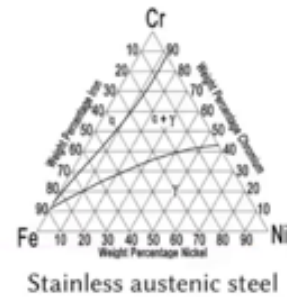
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15m 37s



7.1.3 Ternary plot

- ▶ A ternary plot, ternary graph, triangle plot, simplex plot, or Gibbs triangle is a barycentric plot on three variables which sum to a constant.
- ▶ It graphically depicts the ratios of the three variables as positions in an equilateral triangle.
- ▶ Ternary plots are tools for analyzing compositional data in the three-dimensional case.



products. So you will with two components, you will understand rapidly what changed in comparison with the other situation. So if I have a product x1 and a product x2, you understand that on the ratio, in fact you just you have two products but you just have one degrees of freedom. Is a ratio one in comparison to the total or it could be the ratio in comparison to the other. So in the recipes we are talking, it's all the time a ratio, a concentration, the ratio for the total is we are never talking about the ratio in comparison to the to the other. It could be mass concentration, volume in concentration, anything but it's all the time a concentration. So you understand that with two factors we are in a plane but we are working in fact in a straight line and even a limited straight line because we will work only on between 100% of one and 100% of the other will not go further. So it's in fact we are working on a segment. We have one degrees of freedom and limiting the value of this ratio between one and zero. So when we have three, there are one thing which is very practical. When we have three products we can make ternary plots. It's very common in different in different subjects of science and engineering. They have very different names, you can call them ternary plots, ternary graphs, triangle plots, simplex plots and also for physicists, Gibbs triangle probably, I don't know if he has invented it, but Gibbs was a physicist of the 19th century, probably 19th and start of the 20th century and thermodynamics and so Gibbs. So it's graphically depicts the ratio of the three variables. It's at first approach is complicated to understand but in fact it's present all the situation and it's very well. So it's also present

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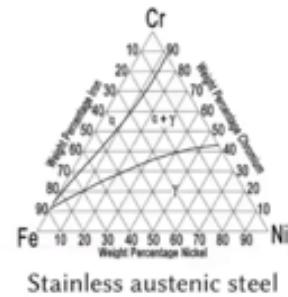
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16m 25s



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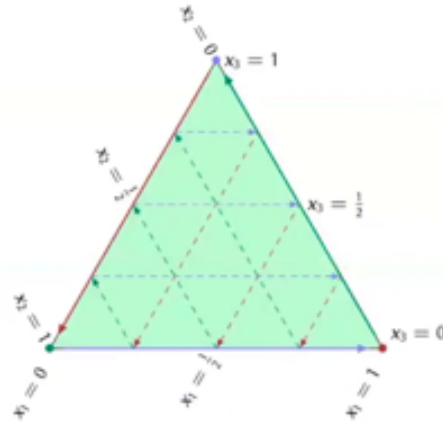
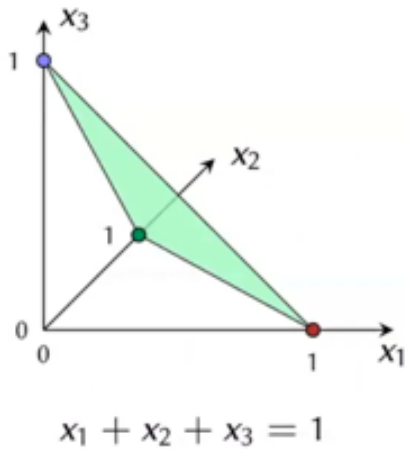
this constraint that any point in the triangle is okay. You can have any concentrations. In all the, in Python, in MATLAB, in latex you have libraries for working with them. Honestly, the routines on MATLAB are not good. They are not official routines and be very careful when you are using it. I will repeat that. Each time I'm using them, I find a few things quite

notes

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7.1.4 Ternary plot : from 3D to 2D

For the case of 3 components, it is usual and useful to draw a ternary diagram.



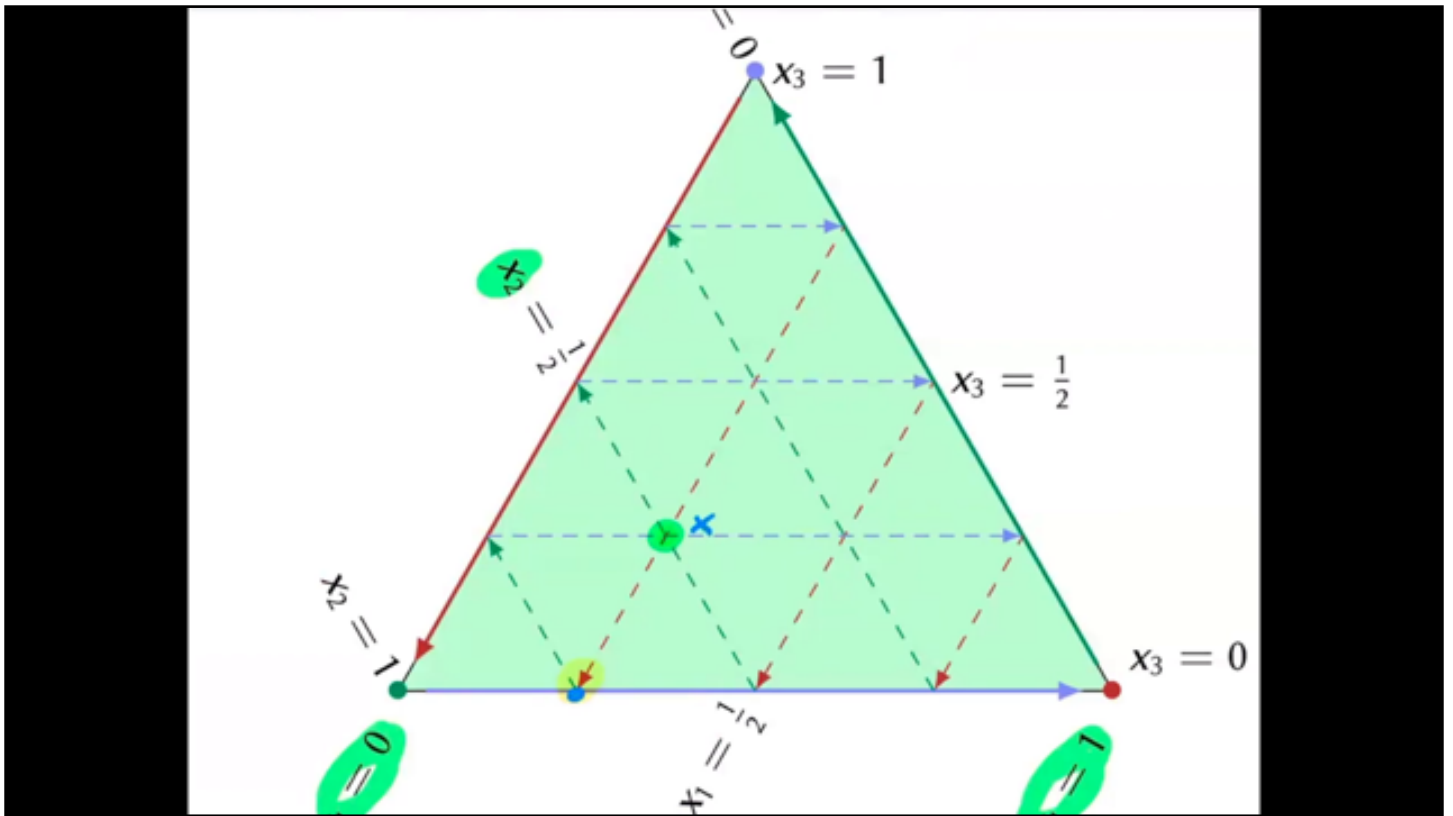
strange with those routines. The routine in latex are very good. I really appreciate latex and in Python, I don't know, you find some but there are a few things you can do by yourself. I will talk perhaps about routines later. When it's more than three-dimension, four-dimension, it's a pyramid, a tetragon, okay, complicated to draw and even to think about. When you have more product, it became very complicated to see what you are doing. Nevertheless, you can apply, you can have model, you can have equation, but it became quite complicated to see it graphically. The two examples that are here, one is about stainless steel. You see the crystallization and it's really, the objective of these two graphics is showing you that even if it's complicated, it's explaining you well what could happen. It's really easy to present what's happened when it's more complicated if you are in orthogonal graphics. It became more complicated. And the other is the soil type. So you can use this graph for making color maps, for making line of iso value or line of border between different behaviors, so very, very, very practical.

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19m 25s





So what is in fact the ternary plot? So the same thing that I present you for two-dimension, but now you have three-dimension, X_1 , X_2 and X_3 . And so the space in which you can move is this green triangle that go between the different 100% of one product and when you diminish. So you have 100% of one when you are here, so you just have this product and the other are not present in the recipe. And when you are diminishing the quantity of the product one, you can increase the concentration of the product two and the product three. So in fact, your space of freedom is this triangle. And now look the triangle which is a side, which is in fact just the same triangle but puts to analyzing it only in two-dimension, but you can look it from one side or the other. I see that not all the algorithm, not all the representation are the same. So I'm used to have the first factor front of you horizontal and having the zero at left and the one at right. And after having the, so sometime having the second on the left side and the third one on the right side, but you can look at the triangle from the other side. So you see that what will be important for reading, it's understanding in which axis that you have to read the value. So how it's work if you have, do I have, no, it's okay. If you have one point, the trick is to understand where to read the three values. So just this year, it's an improvement. I have add a small row for indicating well where to read. So if you want to read the factor one of this point, so imagine that we have this point x here. So here you

notes

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20m 48s



7.1.5 Computing a ternary diagram

MATLAB

No native functions, but a few user defined routines on
<https://ch.mathworks.com/matlabcentral/fileexchange/2299-alchemyst-ternplot>

`ternaxes(12)` create the axis system
`ternplot(A,B,C,'or')` place points in the diagram
`ternpcolor(A,B,Z)` create a colorplot
`ternsurf(A,B,Z)` create a surfaceplot

will read the value of this point, the first coordinate of this point. Here you will read the third coordinate and here you will read the third coordinate. So this point correspond to one quarter for the first one, one, one half, which is here, one half for the second one. And then the third one could be only one quarter. So when you have this type of graph, take time, think to rapidly look at it and see where are factor one, factor two, factor three, where you have to read them and where is the zero because you have other graph when the zero is at left, you have other when the zero is at right. Everything is possible depending on which side you have looked at the triangle. And I've seen the publication, you have everything possible. I don't think there are standards. I believe everybody can do what you want. And the fact of having the zero or one on one side or having the order in which you order your factor will change your graph. Because you can just turn it, but you can also change its side. So it's a mess. So just look at it and try to analyze it when you have such type of graph. So I think that you can compute, you have some routines in MatLamb. So most of you are working with MatLamb. So you can download. I didn't check yesterday, not only somebody wanted to check, but at least last year it was still working. Any problem you write to me. This library proposes you four different very typical routines for one turn for ternary. I don't remember what I put one through is creating a system of access that will draw you the triangle and you can try to think about it. Turn plot. You have a ABC will be the coordinates of your plot. You

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23m 25s



7.1.5 Computing a ternary diagram

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can have only AB and you will calculate the C. So there are the three coordinates of your different points. And here is how you would like to represent the plot. You can have a picolor. I have a lot of I'm not sure how works this routine. I'm using sometimes, but sometimes I feel I have impressions are tricky things. So you can say the position of the points, AB, it will calculate the C. So there are the coordinates of the points and Z will be the altitude of the point. So it will make a color plot of what you have. And honestly, I try with the example I will show you now, but I was not very convinced by the results. And what I'm using with more probability is then surf is creating a surface, a 3D surface over your domain for explaining how is your model based on the points. And I'm not really sure how is really calculating the surface. So when you do that, you better have a lot of have a lot of points for classifying what you can, what should be normal, you should be able to tell I would like a straight plan, I would like a second degree surface or something like that,

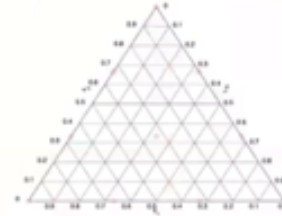
notes

summary

7.1.6 Example with *ternplot()*

MATLAB code

```
ternaxes; % ternary axes
ternlabel('x1','x2','x3'); % placing labels
F=(fullfact([5 5 5])-1)/3; % generating a FFD
index=sum(F,2)==1; % selecting coordinates
E=F(index,:); % essay matrix
ternplot(E(:,1),E(:,2),E(:,3),'or'); % plotting
```



but you cannot do that. It's just making an optimization of the points. Okay, use it, but with really precaution and check what you have and being very critical on the result.

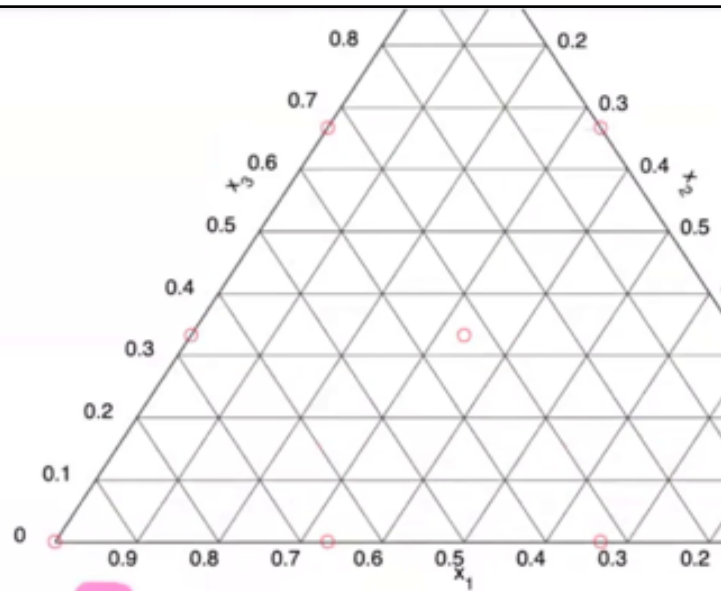
notes

summary

27m 13s



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So I wanted to show you a small example. So I have, this is a small algorithm if you want. So I have used, I have made, what I will do, let's say, so I make 10 place, you have draw when I make the term access, sorry, you have made a triangle. So the result on right is the result on Matlab screen. So you have right me is a different thing. And look what Matlab is doing is putting the,

notes

summary

27m 27s



7.1.6 Example with *ternplot()*

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index=sum(F,2)==1; % selecting coordinates
E=F(index,:); % essay matrix
ternplot(E(:,1),E(:,2),E(:,3),'or'); % plotting
```



if you look at it, is putting the one at left, the reverse I present you in the course.

notes

summary

28m 10s



1.6 Example with *ternplot()*

MATLAB code

```

ternaxes; % ternary axes
ternlabel('x1','x2','x3'); % placing labels
F=(fullfact([5 5 5])-1)/3; % generating a FFD
index=sum(F,2)==1; % selecting coordinates
E=F(index,:); % essay matrix
ternplot(E(:,1),E(:,2),E(:,3),'or'); % plotting

```



To define the label. So we have introduced this element. And for making them beautiful, you can have an handle and after you can move them for putting them in a other position and changing the font and things like that. After I have,

notes

summary

28m 17s



notes

28m 39s



7.1.6 Example with *ternplot()*

MATLAB code

```
ternaxes; % ternary axes
ternlabel('x1','x2','x3'); % placing labels
F=(fullfact([5 5 5])-1)/3; % generating a FFD
index=sum(F,2)==1; % selecting coordinates
E=F(index,:); % essay matrix
ternplot(E(:,1),E(:,2),E(:,3),'or'); % plotting
```



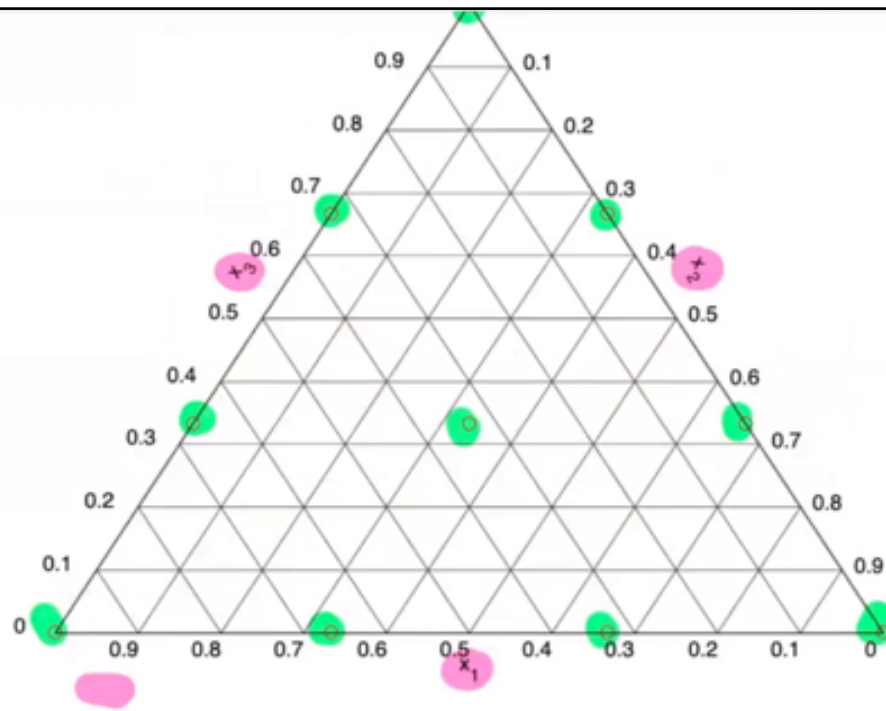
look at the points, the points are, my points are here, here, here, here, here, here, here, here,

notes

summary

28m 51s





here, here, here. So I wanted to put the point in a specific place. But so I have created with F full factorial of five levels in a square one, zero to one. But when I do that, I get a lot of points. And then a lot of points were not in my triangle. So after I check, look, this is a way in MATLAB for selecting coordinates answering to a condition. So I say, tell me the position in F2. It will give me an F2. So that the sum of the horizontal lines, the coordinates of my point is equal to one, because I just wanted points that correspond to 100. So to be recipes. And after I have a matrix of experiments, which is only those points. So it's why I say E equal, F was a big matrix. And I just wanted the one answering yes to my condition, the sum of the coefficient, the sum of the coordinates are one. And after I have used 10 plots and we have so I give the coordinates in the key that are called A, B, A, B, C, etc. So I give him the coordinate and I say, I want circle and red. So and they have produced me this

notes

summary

29m 3s



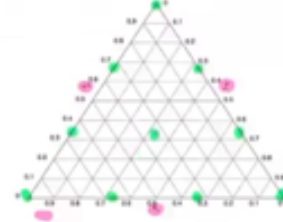
7.1.6 Example with *ternplot()*

MATLAB code

```

ternaxes; % ternary axes
ternlabel('x1','x2','x3'); % placing labels
F=(fullfact([5 5 5])-1)/3; % generating a FFD
index=sum(F,2)==1; % selecting coordinates
E=F(index,:); % essay matrix
ternplot(E(:,1),E(:,2),E(:,3),'or'); % plotting

```



type of drawings. So next week, we will look at it. We need one hour and perhaps one hour and a half. But after we have some time for talking about the course and having your feedback too, also. So be prepared next week to give me your feedback and what you appreciate, what you less appreciate, whereas difficulty.

notes

summary

30m 37s

