Modelling and design of experiments

Chapitre 7: Mixture designs

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7.1.1 Specificity of mixture spaces

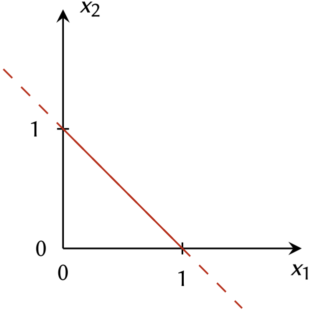
- A mixture space is considered when the factors x_i are fractions of a whole and that the increase of one factor implies the decrease in proportion of one or more other factors.
- This situation then implies in addition to the model $f(\vec{x})$ to be determined, two other conditions :
    1. a constant sum : $\sum_{i=1}^{q} x_i = 1$
    2. positive values $x_i \geq 0$

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 :

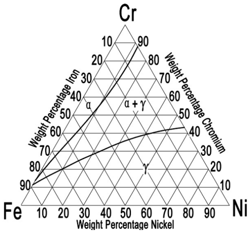
$$x_1 + x_2 = 1$$

- The experimental space has one degree of freedom only

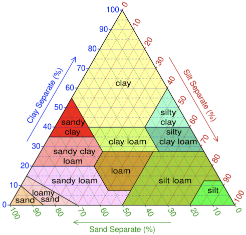


7.1.3 Ternary plot

- 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.



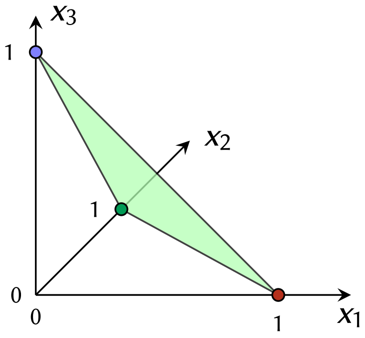
Stainless austenic steel



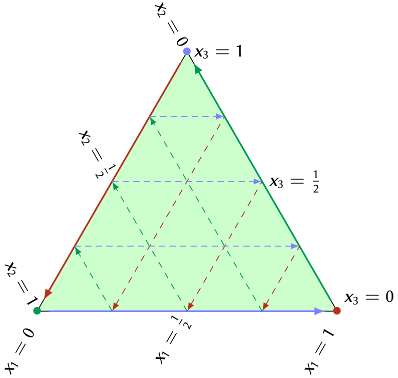
Soil types

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.



$$x_1 + x_2 + x_3 = 1$$



7.1.5 Computing a ternary diagram

MATLAB

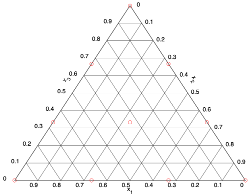
No native functions, but a few user defined routines on
`https://ch.mathworks.com/matlabcentral/fileexchange/2299-alchemyst-ternplot`

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

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
```



7.1.7 Example : Optimization of a greenhouse

7.1.8 Optimization of a greenhouse : mindmap

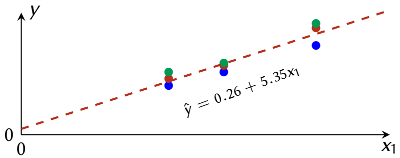
Greenhouse

- **Objective :** Model the behaviour of a greenhouse during the cold season in relation with the ratio of glass and wall
- **Investigation :** Observational study based on in-situ monitoring
- **Factors :**
  (1) Surface of wall
  (2) Surface of window
- **Responses :**
  (1) Average of overheated hours by day in one month in-situ monitoring in three buildings during the cold season
  (2) Average vote about the comfort in the greenhouse
- **Models :**
  (1) Linear model
  (2) Quadratic model
- **Strategy :** In-situ measurements and questionnaires

7.1.9 Optimization of a greenhouse : data

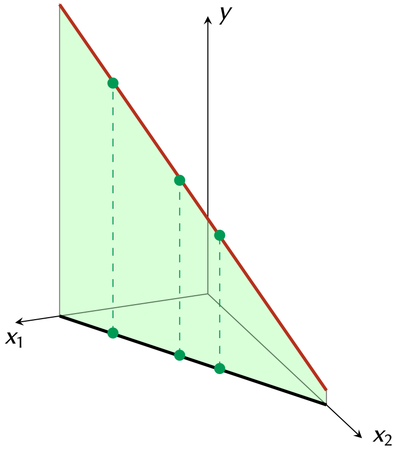
Table – Average overheating hours ($T_{in} \geq 25^oC$)

Building	A	B	C
Window	40%	55%	80%
D	2.2 hrs/D	2.8 hrs/D	4 hrs/D
J	2.5 hrs/D	3.1 hrs/D	4.8 hrs/D
F	2.8 hrs/D	3.2 hrs/D	5 hrs/D



7.1.10 Optimization of a greenhouse : model

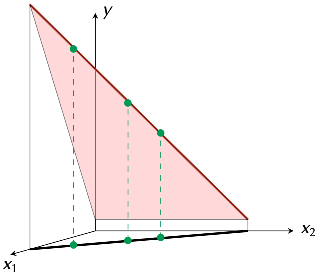
Here is the solution in the plane $x_1 + x_2 = 1$

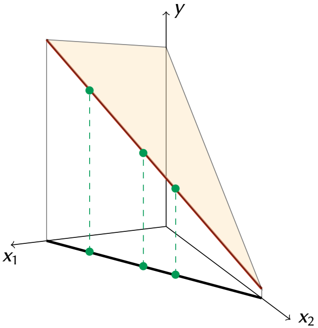


7.1.11 There are an infinity of solutions

$\hat{y} = 0.26 + 5.35x_1 = 0.26(x_1 + x_2) + 5.35x_1 = 5.61x_1 + 0.26x_2$

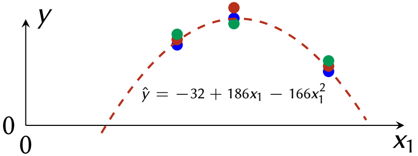
$\hat{y} = 5 + 5.35x_1 - 4.74(x_1 + x_2) = 5 + 0.61x_1 - 4.74x_2$



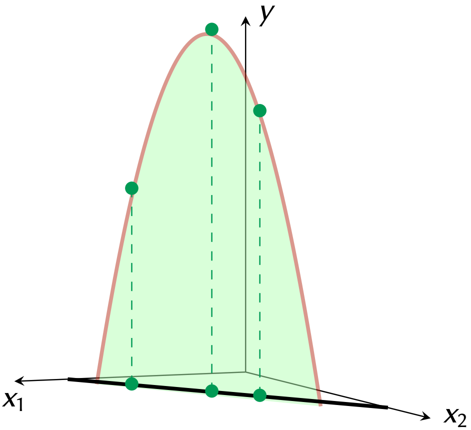


7.1.12 Average votes about the comfort

Building	A	B	C
Window	40%	55%	80%
P1	15	20	10
P2	16	22	11
P3	17	19	12

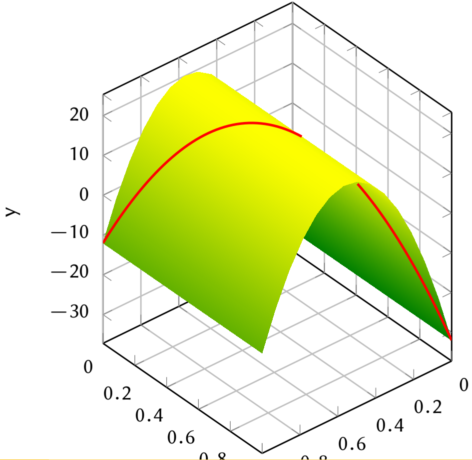


7.1.13 Solution in the plane $x_1 + x_2 = 1$



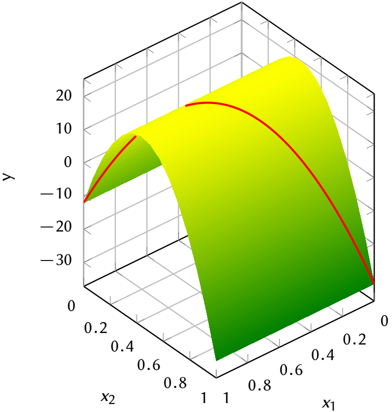
7.1.14 A possible model in 3 dimensions

- The function $y = -32 + 18x_1 - 166x_1^2$ can be interpreted as a paraboloid in the 3D space $x_1 x_2 y$
- But an infinity of functions have the same intersection with the vertical plane $x_1 + x_2 = 1$



7.1.15 Here is another possible model

$$
\begin{aligned}
y &= -32 + 18x_1 - 166x_1^2 \\
&= -32 + 186(1 - x_2) - 166(1 - x_2)^2 \\
&= -12 + 146x_2 - 166x_2^2
\end{aligned}
$$



7.2.1 Scheffé's and slack models

- The reduction to a $(N_{fact} - 1)$ dimension experiment space, due to the additional equation $\sum_{i=1}^{q} x_i = 1$, has the consequence that several models allows to model a given response.
- The imposed correlation between the factors reduces the rank of the essay matrix E of one unit.
- A *canonical* model is needed : a unique representation for the different models that represent the same response
- There are several possible choices
  - Scheffé's models (models without an intercept)
  - Slack models (models with an intercept)

7.2.2 Scheffé's linear mixture model

- Let's start with a standard linear model of rank $(q+1)$:

$$y = a_o + \sum_{i=1}^{q} a_i x_i$$

- Let's introduce, at the level of the constant a_o, the proportionality constraint $\sum_{i=1}^{q} x_i = 1$
- The Scheffé's model (of rank q) is then :

$$y = \sum_{i=1}^{q} (a_o + a_i) x_i = \sum_{i=1}^{q} \beta_i x_i$$

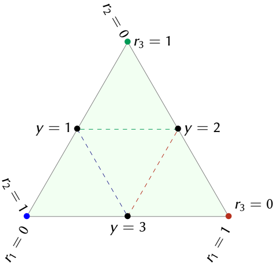
- With the Scheffé's linear coefficients $\beta_i = (a_o + a_i)$

7.2.3 Example of a Scheffé's linear model

1. A recipe is made with three ingredients x_1, x_2 and x_3 so that $x_1 + x_2 + x_3 = 1$
2. Essays have been made at the middles of the vertices of the ternary scheme. The output y is a KPI of the process.

x_1	x_2	x_3	y
0.5	0.5	0	2
0.5	0	0.5	3
0	0.5	0.5	1

3. Determine the coefficients of the Scheffé's linear model

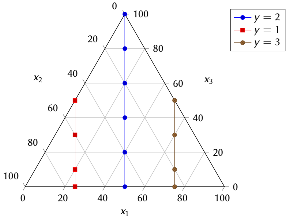


7.2.4 Identification of a Scheffé's linear model

Model : $Y = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon$

Linear system :

$$\begin{pmatrix} 2 \\ 3 \\ 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} \Leftrightarrow \begin{cases} \beta_1 + \beta_2 = 4 \\ \beta_1 + \beta_3 = 6 \\ \beta_2 + \beta_3 = 2 \end{cases}$$



Solution :

$$\begin{cases} \beta_3 = 2 \\ \beta_2 = 0 \\ \beta_1 = 4 \end{cases} \quad \Rightarrow \quad \hat{Y} = 4x_1 + 2x_3$$

Isolines :

$$\begin{cases} x_1 = x_1 \\ x_2 = x_1 - \frac{y}{2} + 1 \\ x_3 = \frac{y}{2} - 2x_1 \end{cases}$$

7.2.5 Quadratic Scheffé's model

- The standard quadratic model of rank $(q+1)(q+2)/2$ is :

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

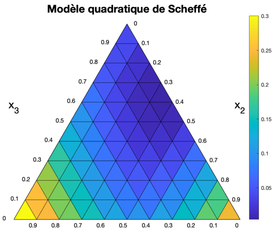
- The constraint of proportionality allows to write :

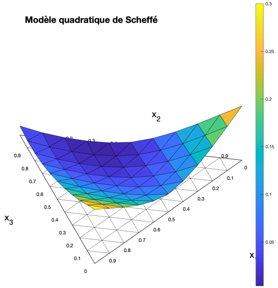
$$\begin{cases} a_o = a_o\, 1 = a_o \sum_{i=1}^{q} x_i = \sum_{i=1}^{q} a_o x_i \\ a_{ii}\, x_i^2 = a_{ii}\, x_i \left(1 - \sum_{j \neq i}^{q} x_j\right) \end{cases}$$

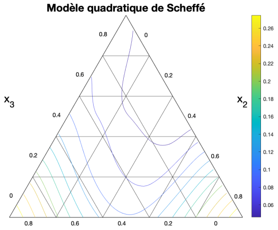
7.2.6 Quadratic Scheffé's model (2)

- When recombining the coefficients the quadratic Scheffé's model of rank $q(q+1)/2$ is then

$$y = \sum_{i=1}^{q} \beta_i \, x_i + \sum_{i<j}^{q} \beta_{ij} \, x_i \, x_j$$







7.2.7 Cubic Scheffé's model

- The standard cubic model is :

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

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

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

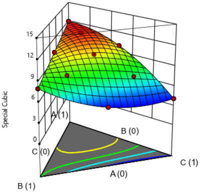
- Its rank is $q(q+1)(q+2)/3!$
- Truncated form if $\gamma_{ij} = 0$ (allows to diminish the number of runs)

7.2.7 Example of cubic Scheffé's model

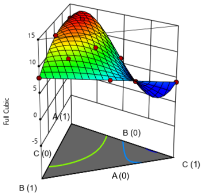
$$y = 12x_2 + 8x_2 + 4x_3 + 8x_1x_3 - 8x_2x_3 + 54x_1x_2x_3$$

$$y = 2x_1 + 8x_2 + 4x_3 + 8x_1x_2 - 8x_1x_3 + 54x_1x_2x_3 + 48x_1x_3(x_1 - x_3)$$

Scheffé Special cubic



Scheffé full cubic



7.2.8 Slack model

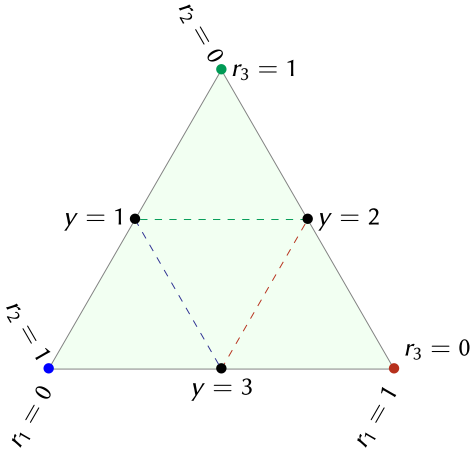
- It is in neglecting one factor in the model. It represents a risk if the neglected factor is active. So it is better to reserve this for factors having only linear effect.
- SV means Slack Variable
- Full linear SV model

$$y = a_o + \sum_{i=1}^{q-1} a_i x_i$$

- Full quadratic SV model

$$y = a_o + \sum_{i=1}^{q-1} a_i x_i + \sum_{i=1}^{q-1} a_{ii} x_i^2 + \sum_{i=1}^{q-2} \sum_{j=i+1}^{q-1} a_{ij} x_i x_j$$

7.3.1 Constraints

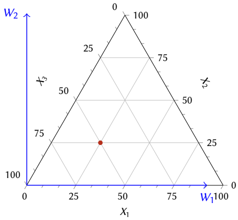


7.3.2 Transformation ternary to Cartesian

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

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

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

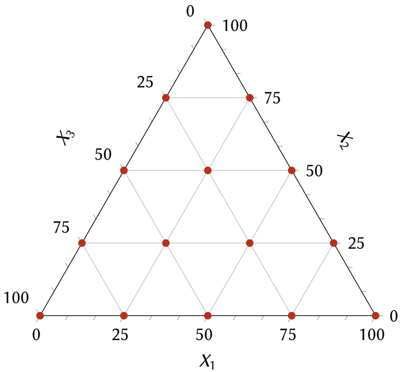


7.4.1 Simplex lattice design {q,m }

Factorial design for q components with levels $\left(\frac{0}{m}, \frac{1}{m}, \ldots, \frac{m}{m}\right)$

- Example {q=3,m=4}
- The levels are $\left(0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1\right)$
- The matrix of experiments

$$\begin{pmatrix} 1 & 0 & 0 \\ 0.75 & 0.25 & 0 \\ 0.75 & 0 & 0.25 \\ 0.5 & 0.5 & 0 \\ 0.5 & 0 & 0.5 \\ 0.5 & 0.25 & 0.25 \\ 0.25 & 0.75 & 0 \\ 0.25 & 0 & 0.75 \\ 0.25 & 0.5 & 0.25 \\ 0.25 & 0.25 & 0.5 \\ 0 & 1 & 0 \\ 0 & 0.75 & 0.25 \\ 0 & 0.5 & 0.5 \\ 0 & 0.25 & 0.75 \\ 0 & 0 & 1 \end{pmatrix}$$



7.4.2 Simplex lattice design

$$N_{exp} = \binom{q+m-1}{m} = \frac{(q+m-1)!}{m!(q-1)!}$$

Number of points per design

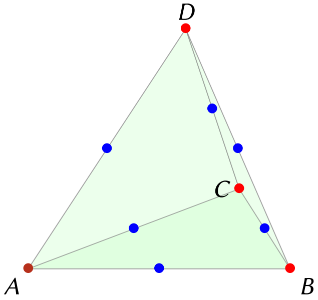
q	m		
	2	3	4
3	6	10	15
4	10	20	35
5	15	35	70
6	21	56	126
7	28	84	210

Number of coefficients per model

q	linear	quad-ratic	special cubic	full cubic
3	3	6	7	10
4	4	10	14	20
5	5	15	25	35
6	6	21	41	56
7	7	28	63	84

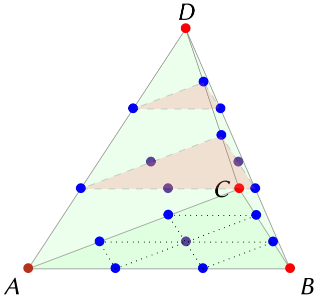
7.4.3 Simplex lattice design {4,2 }

- $N_{exp} = 10$
- Sufficient for a quadratic model
  $$y = \sum_{i=1}^{q} \beta_i \, x_i + \sum_{i<j}^{q} \beta_{ij} \, x_i \, x_j$$
- But No point within the domain : no full mixture



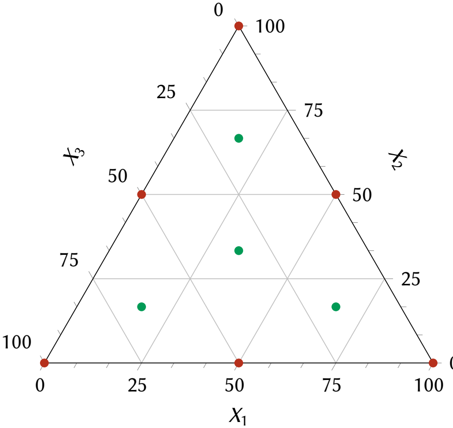
7.4.4 Simplex lattice design {4,3 }

- $N_{exp} = \binom{4+3-1}{3} = \binom{6}{3} = 20$
- Sufficient for a full cubic model
- But No point within the domain : no full mixture
- We need another type of design to bu sure to enter in the domain



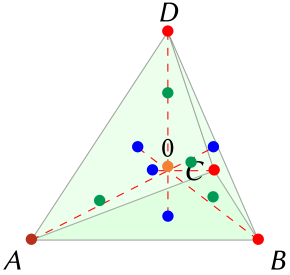
7.4.5 Simplex response surface

- If $m < q$ there is no full mixture
- Then designs {q,2 } have to be completed with $q + 1$ points
- One point at the center $(1/q, 1/q, \ldots)$
- q points at he middle of the distance between the center and the vertices (axial check blends)
- This has the advantage of offering additional degrees of freedom



7.4.6 Simplex screening design

- As its name suggests, it is a question of determining the variables that can be eliminated from the problem.
- The design is composed by
  - the vertices - q points
  - the central point - 1 point
  - the points in the middle of the distance from the center to the vertices (axial check blends) - q points
  - the end points - q points
- With 3 factors, it is the same design as the Simplex response surface



7.4.7 Conclusions

- A **comprehensive overview** of important approaches in mixture design.
- These approaches offer a versatile toolkit for tackling diverse mixture design problems allowing **flexibility and adaptability**.
- They reduce the need for extensive experimentation, saving time and resources, providing robust solutions less susceptible to variability and uncertainty : **efficiency and robustness**
- **Improved Decision-Making** : enhance our understanding of the relationships between components, enabling process adjustments and improving product performance.