New experimental designs for mixture problems

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Formulation

….. drugs, foods and drinks, polymer plastics, ceramics, glass, textile fiber blends, fertilizers, paints, ….

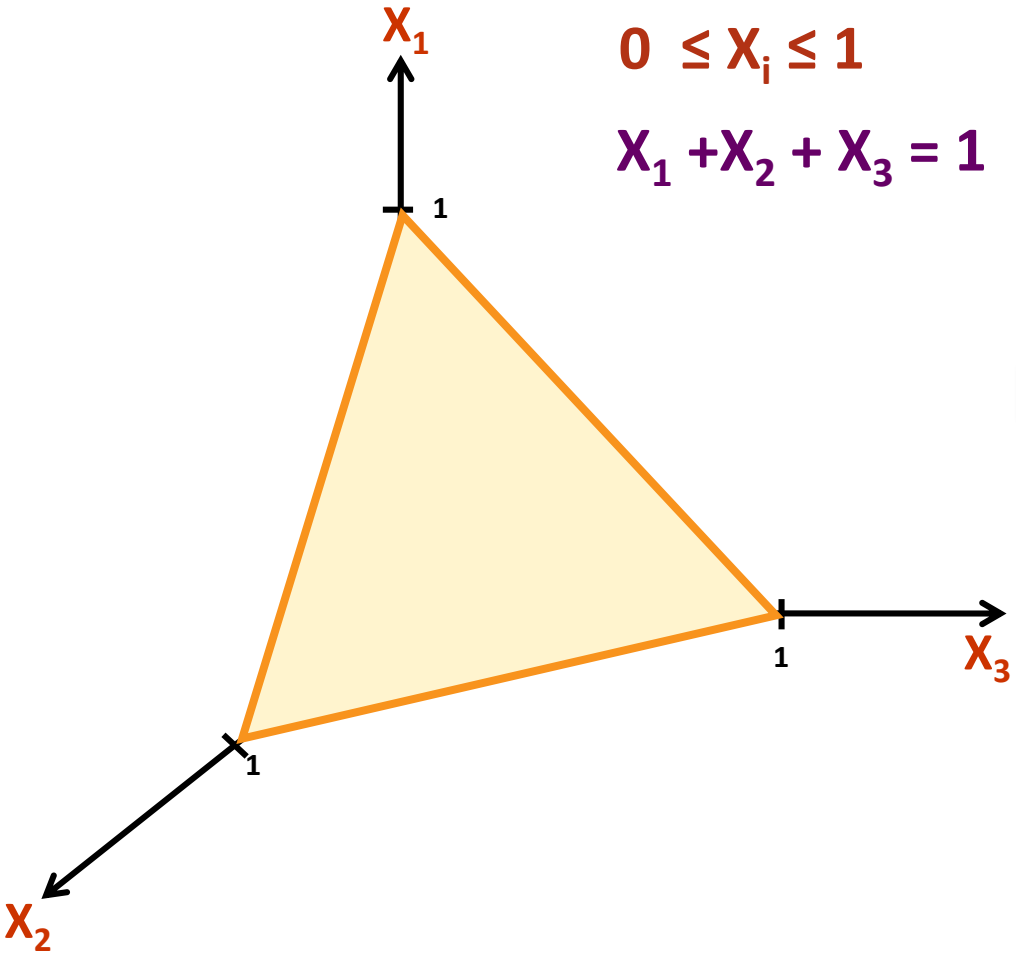
Y (*Output Variables*) = **f(component proportions)**

The **INPUT VARIABLES** of the experimental design are the **proportions** of different mixture **components**

X_i : proportion of the component i

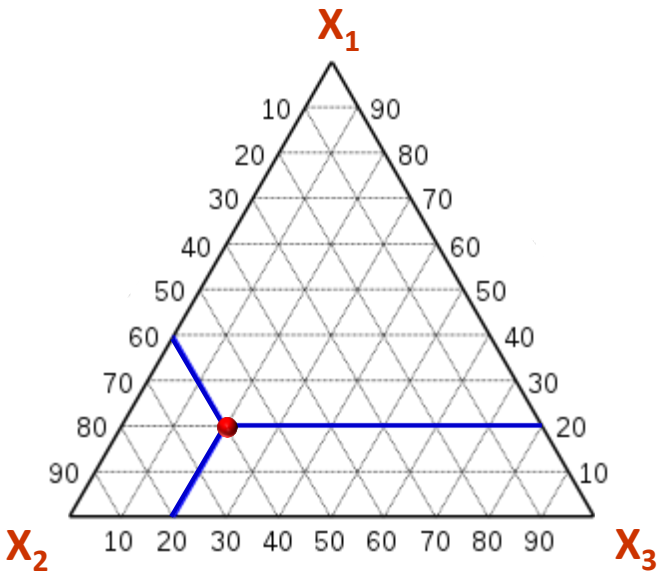
Formulations obtained by mixing two or more ingredients (components)

Formulation



$$0 \leq X_i \leq 1$$

$$X_1 + X_2 + X_3 = 1$$



Domain = simplex

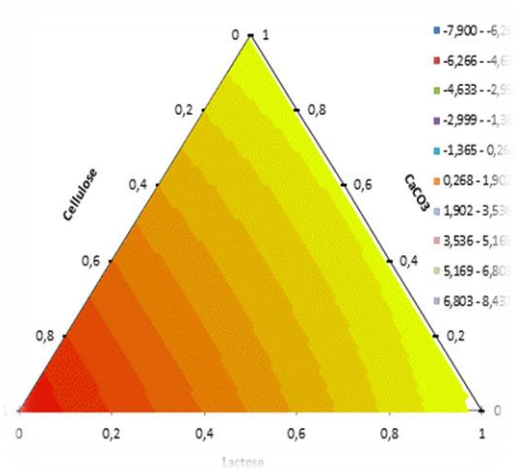
Experimentation

To search for the optimum of one or several responses in the domain of interest

To know, in the whole experimental domain, the value of the experimental response(s)

Mathematical Model

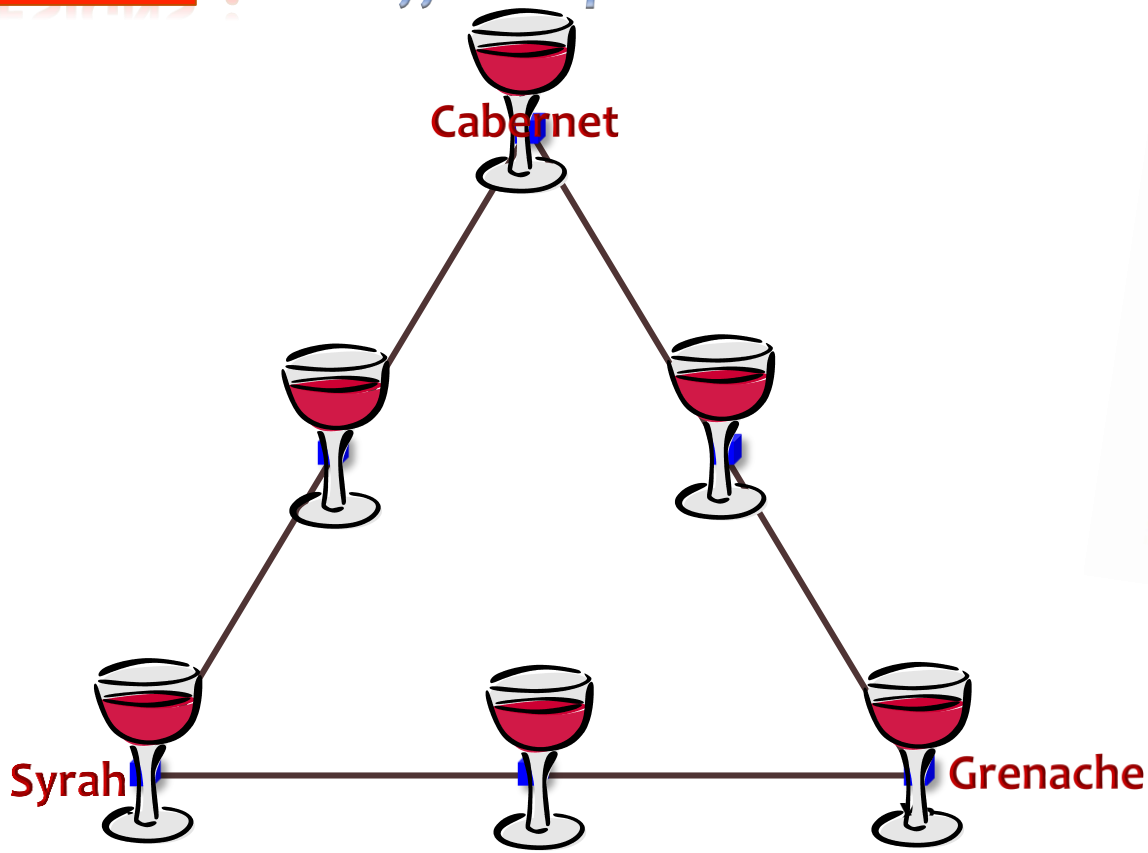
$$Y = f(X_i)$$



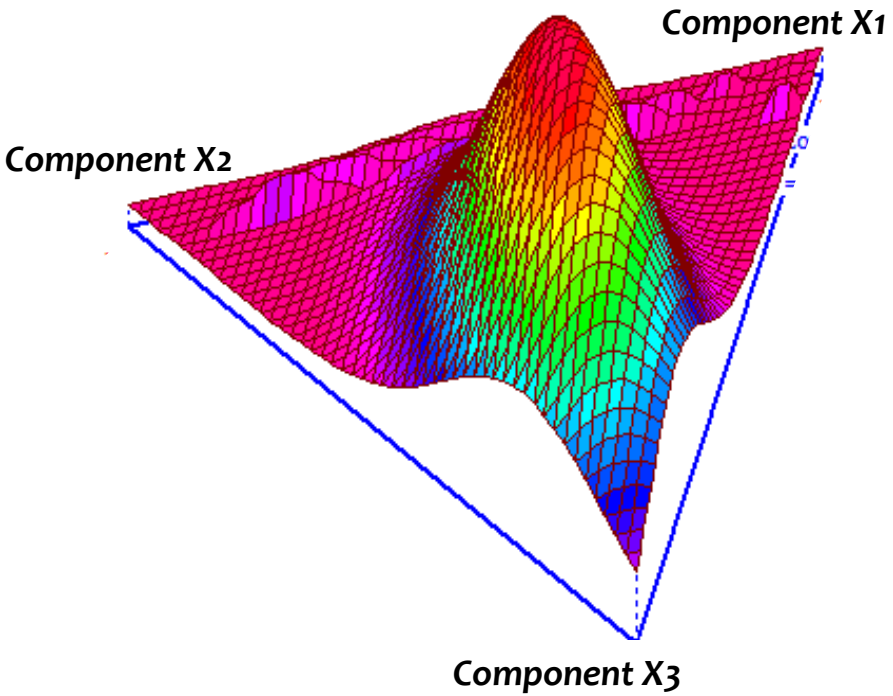
Mixture :

Empirical model : $Y = b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3$

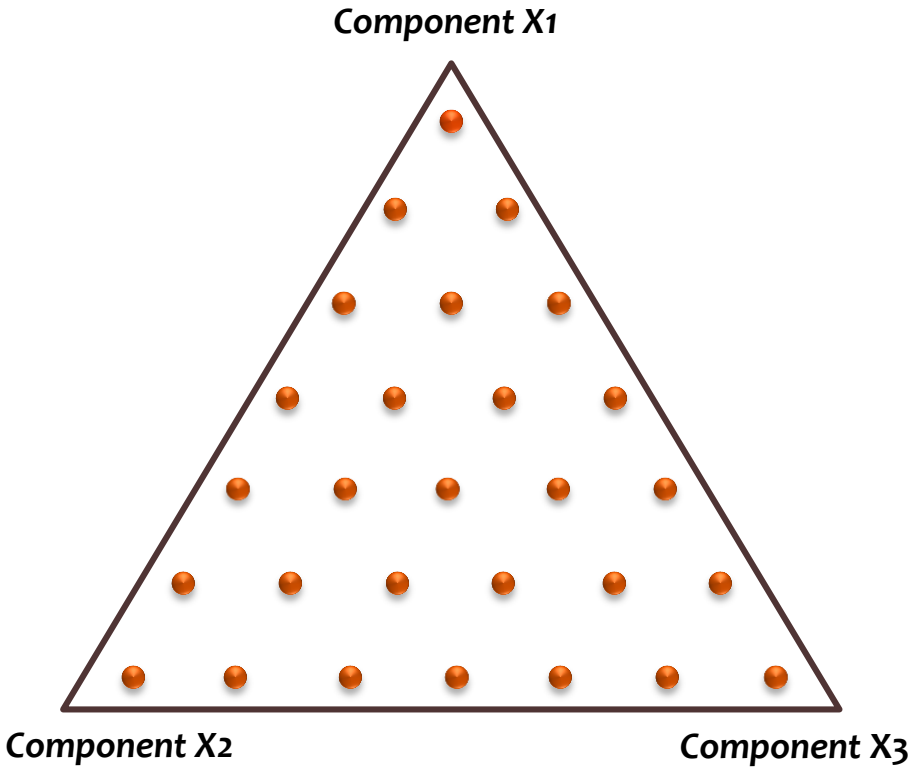
OPTIMAL DESIGNS : *Scheffé Simplexe lattice*



Complex response surface :



Space Filling Design



SFD : Space Filling Design

A Space-Filling design (SFD) aims to uniformly spread the experimental points in the domain of the inputs

Some space-filling designs ….

- **Latin Hypercubes** : *Random LHS, Maximin LHS, Improved LHS*
  projection criteria
- **Low discrepancy sequences** : *Halton, Hammersley, Faure, Sobol, …*
- **Minimax designs** : *maximum distance between 2 points*
- **Dmax designs** : *maximum entropy*
- **Strauss designs** : *repulsion principle*
- **WSP selection algorithm**

Mixture designs

WSP algorithm : selection algorithm

Generate a set of candidate points

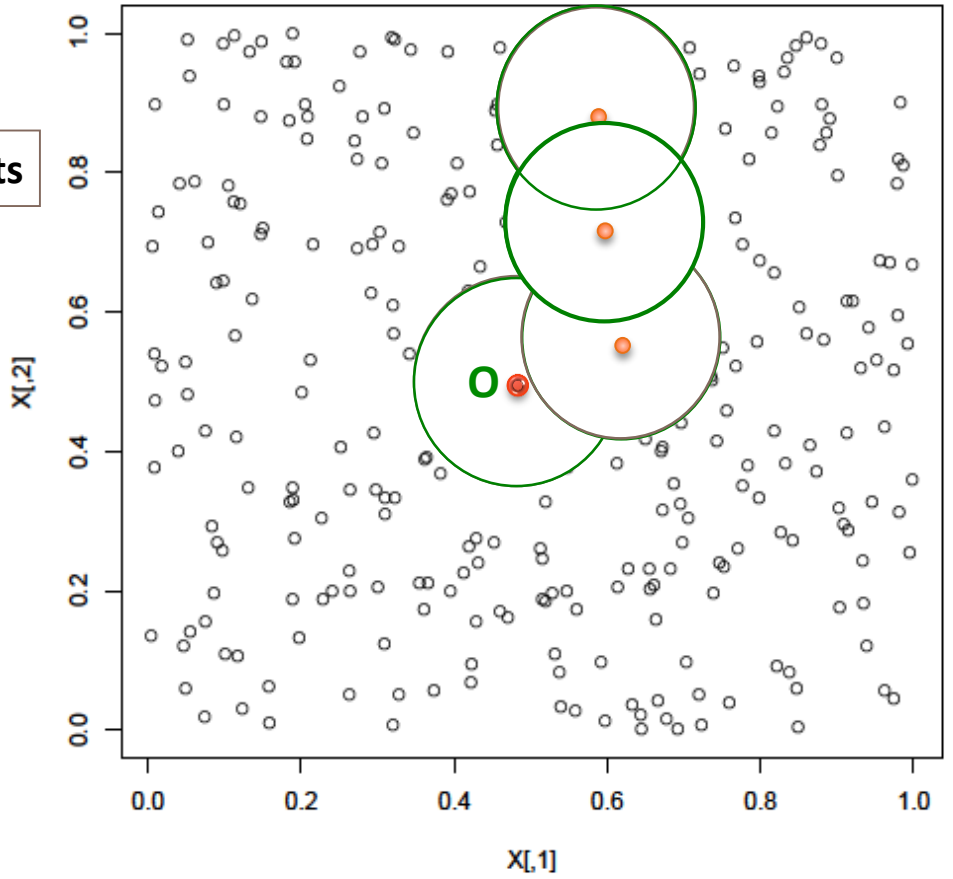
calculate the distances (D_{ij}) matrix of the N points

choose an initial point O and a distance d_{min}

eliminate the points I such as : $D_{OI} < d_{min}$

the point O is replaced by the nearest point among the remaining points

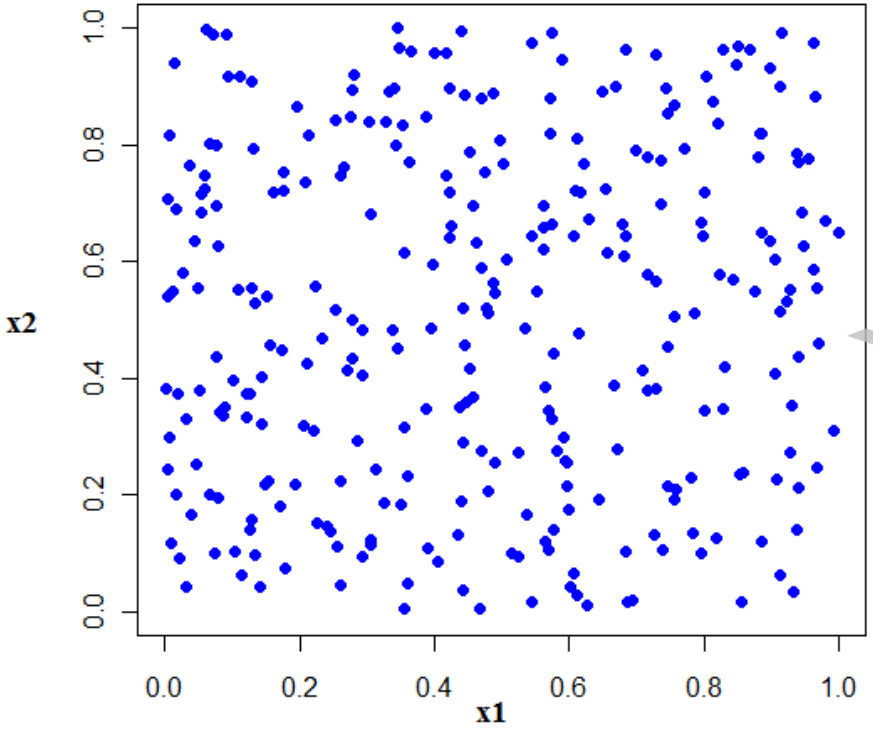
repeat the procedure until there are no more points to choose



WSP Algorithm :

set of candidate points

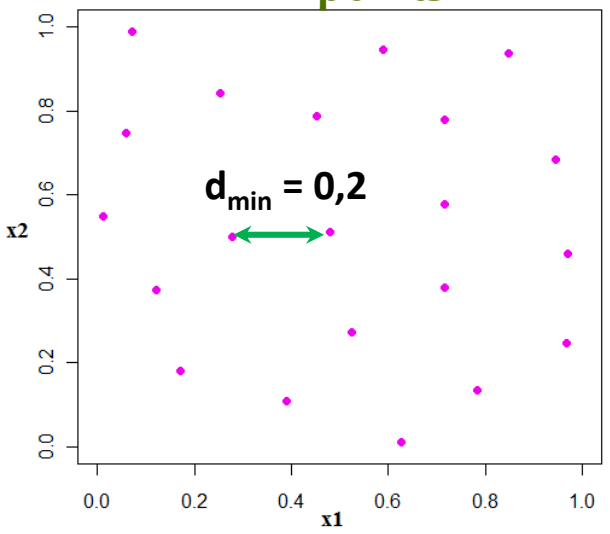
N = 300



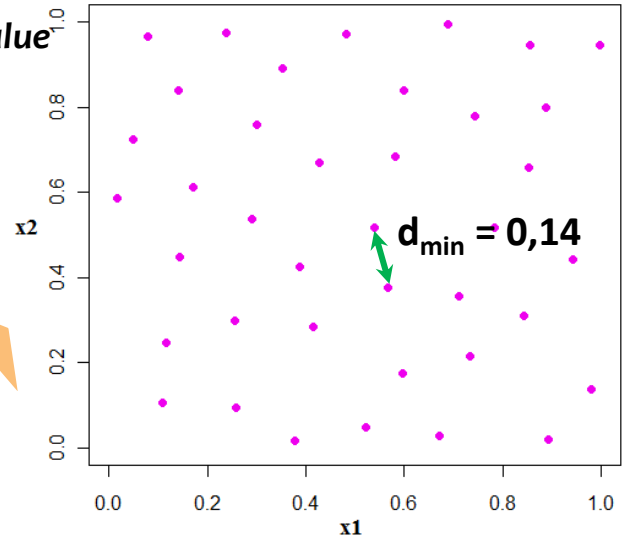
WSP

for a given value of d_{min}

N=20 points



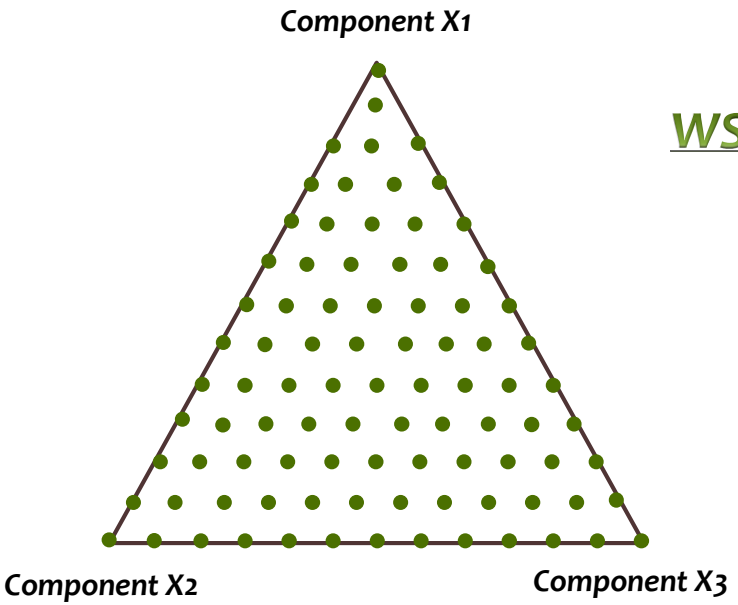
N=40 points



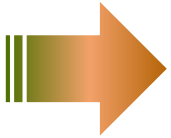
Mixture designs

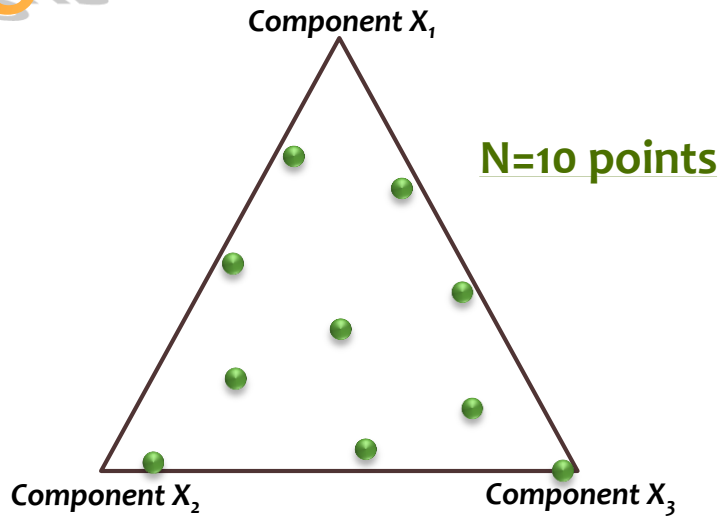
WSP Algorithm for mixture :

Generate a set of candidate points in the mixture simplex domain

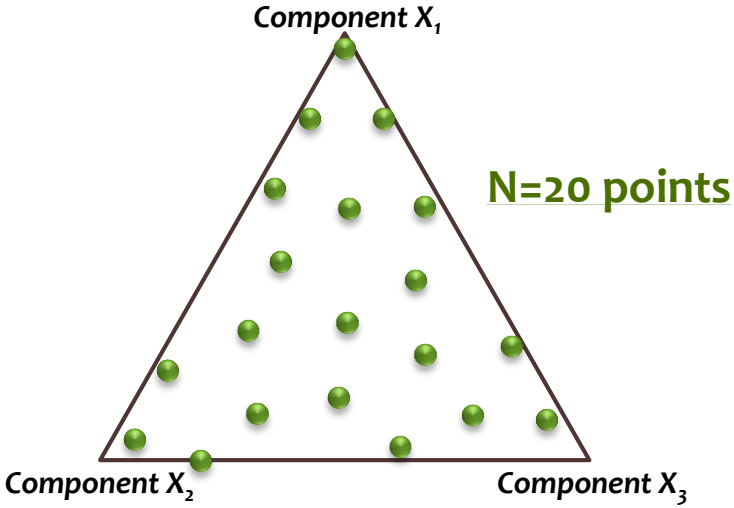


WSP algorithm





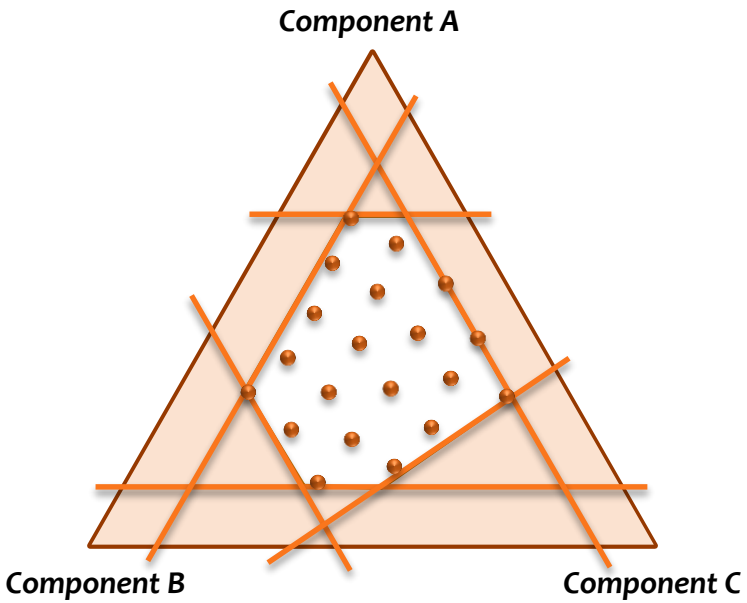
N=10 points

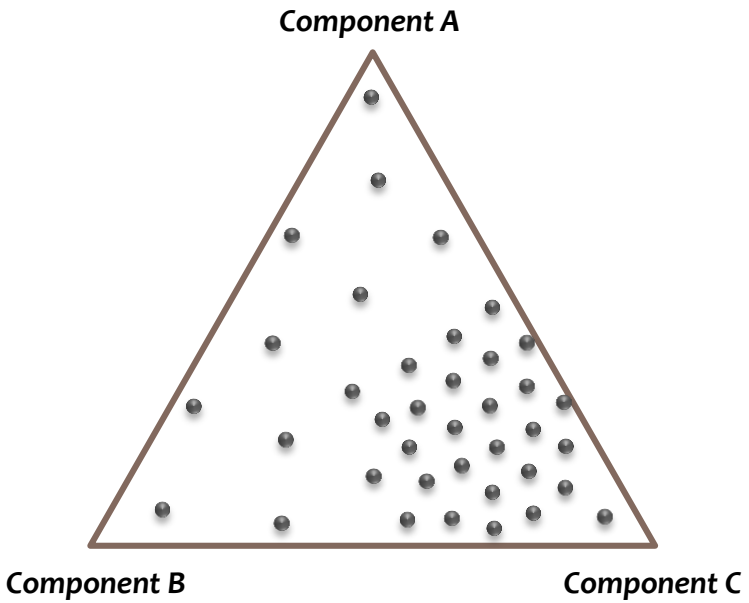


N=20 points

- Specific experimental constraints
- Increasing density in a zone of particular interest

Adaptative WSP algorithm



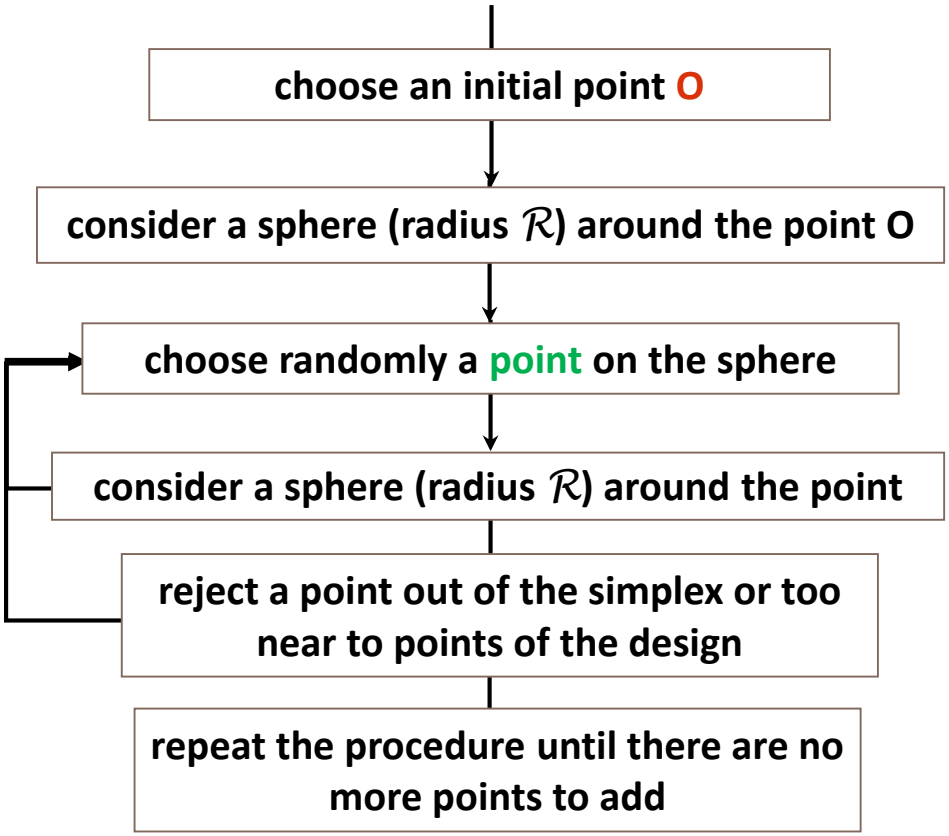


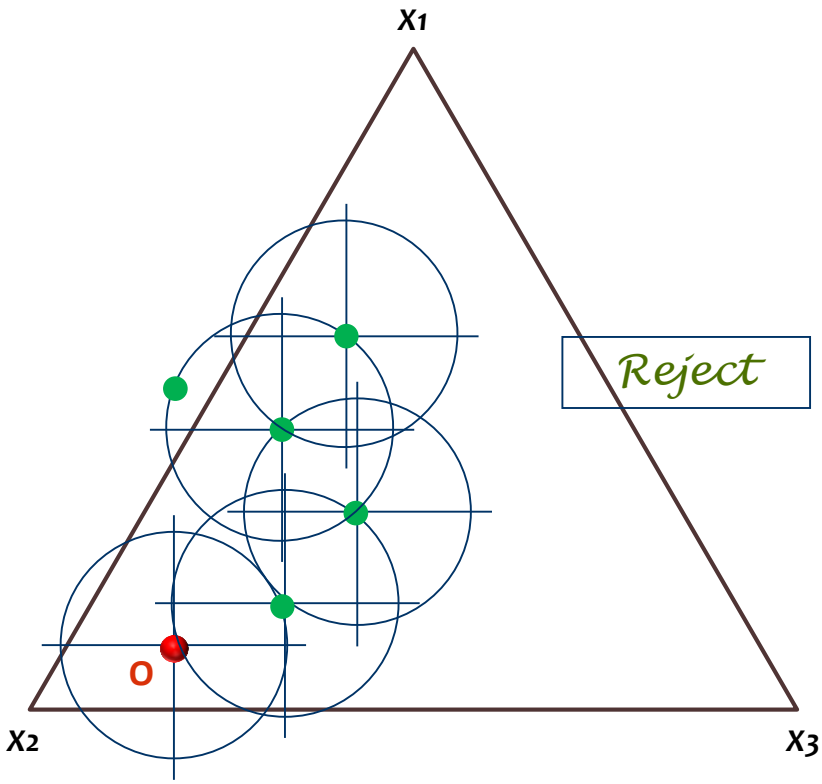
Beal A., Claeys-Bruno M., Sergent M., Constructing space-filling designs using an adaptive WSP algorithm for spaces with constraints Accepted in Chemometrics and Intelligent Laboratory System, 2014

Mixture designs

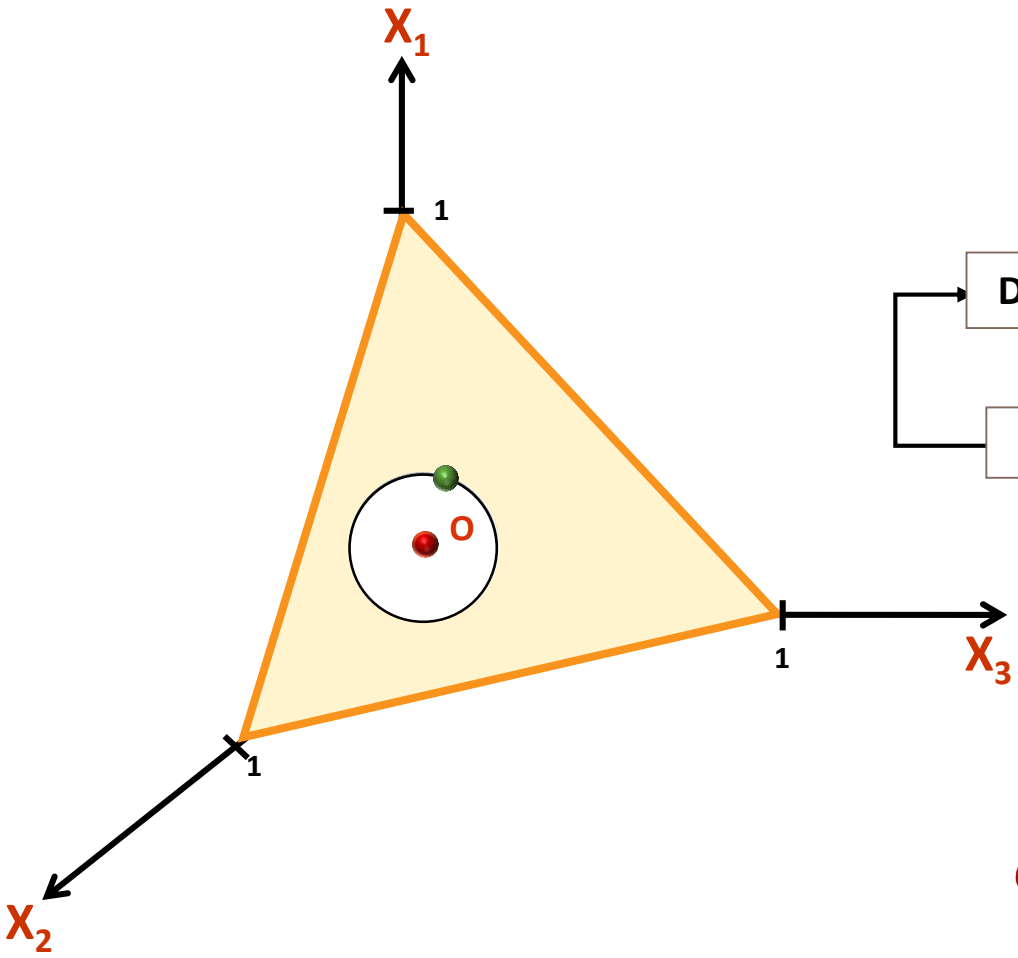
Step by Step algorithm :

A set of N points is built by iteration from an initial point, by adding points at a distance $\mathcal{R}$ of the points already in the design





Step by Step algorithm :



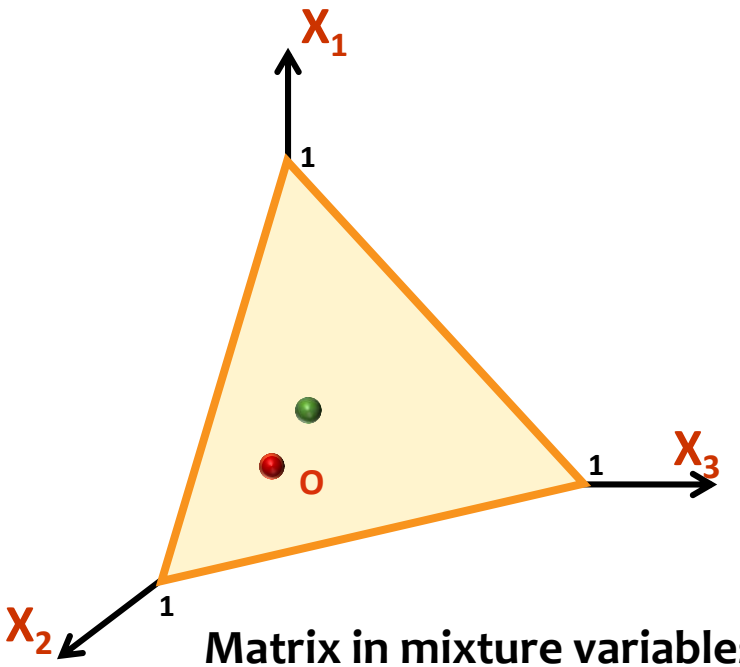
choose an initial point O

Draw a sphere (radius $\mathcal{R}$) around the point O

choose randomly a point on the circle

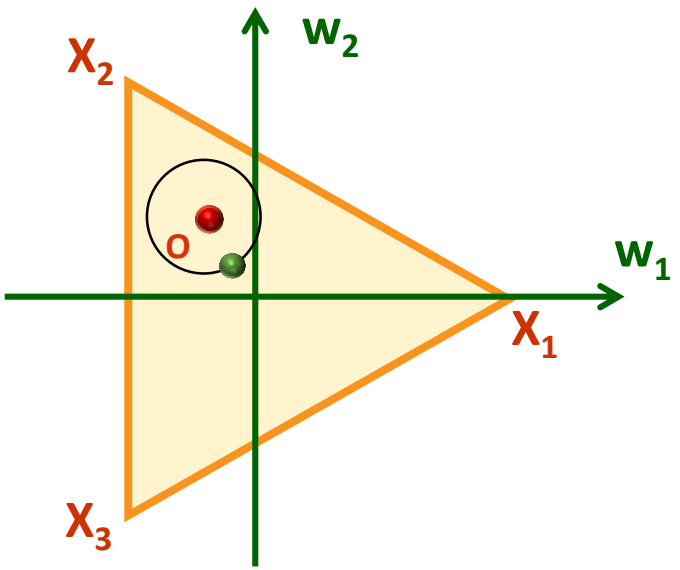
q, number of components

Cornell algorithm *: transformation of a classical design in an independant variables space to a mixture design around an interesting point.*



Matrix in mixture variables

X



Matrix in orthogonal variables

W

$$W = (q-1)\{qX - J\}\theta$$

with , θ *: orthogonal matrix*

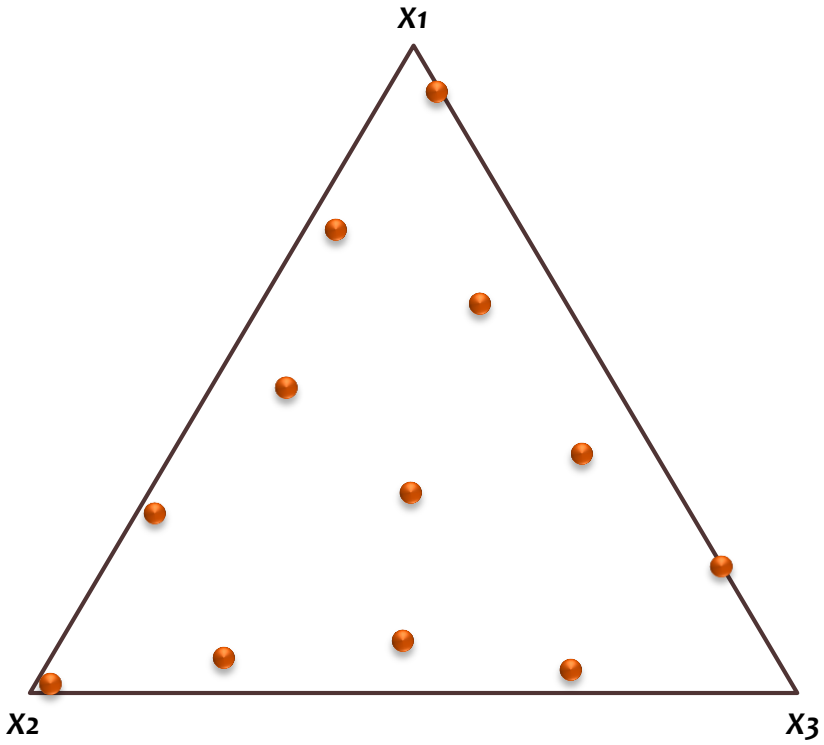
$$X = cWT_1'H + x_0'$$

with , T *: rotation matrix*

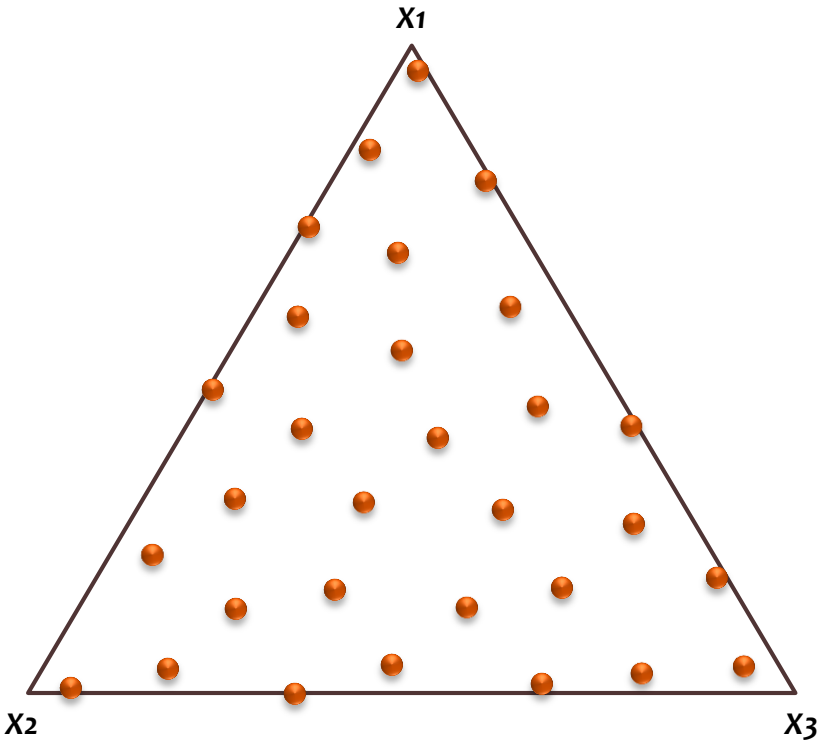
x_o *: point O*

Mixture designs

Step by Step algorithm :



N = 12 points

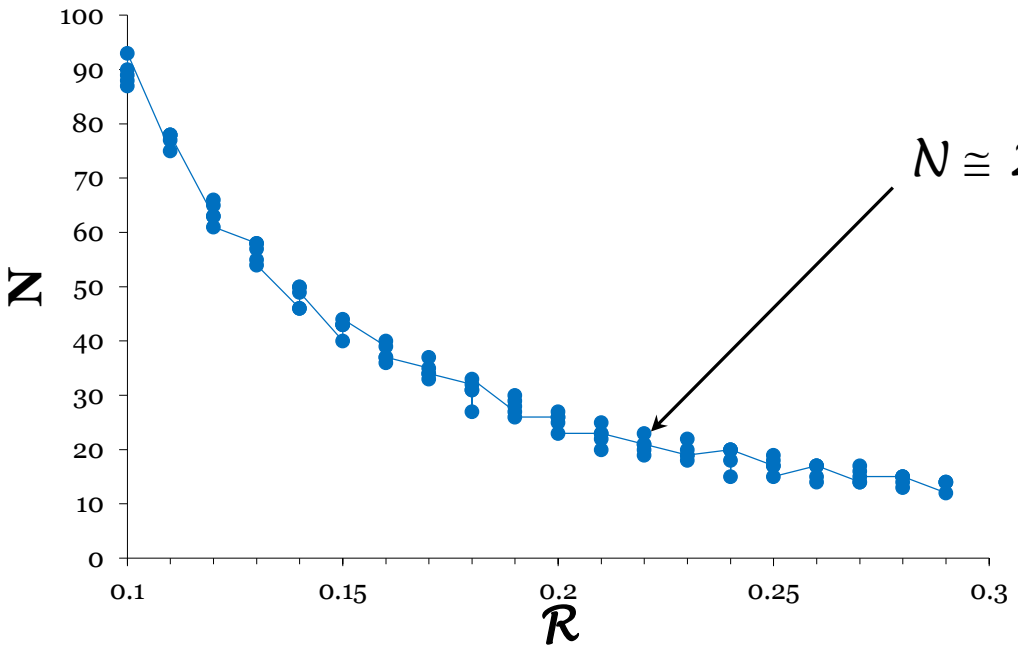


N = 30 points

Space Filling Design

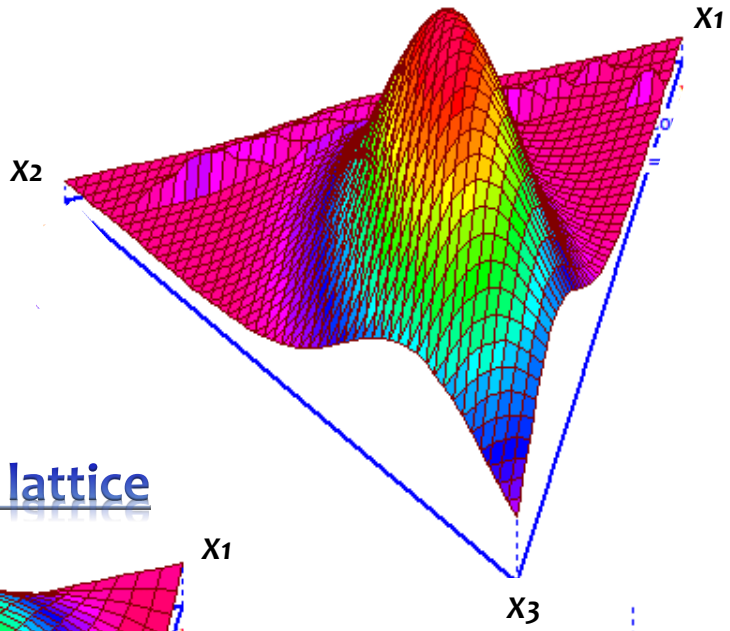
Step by Step algorithm :

Stochastic choose !

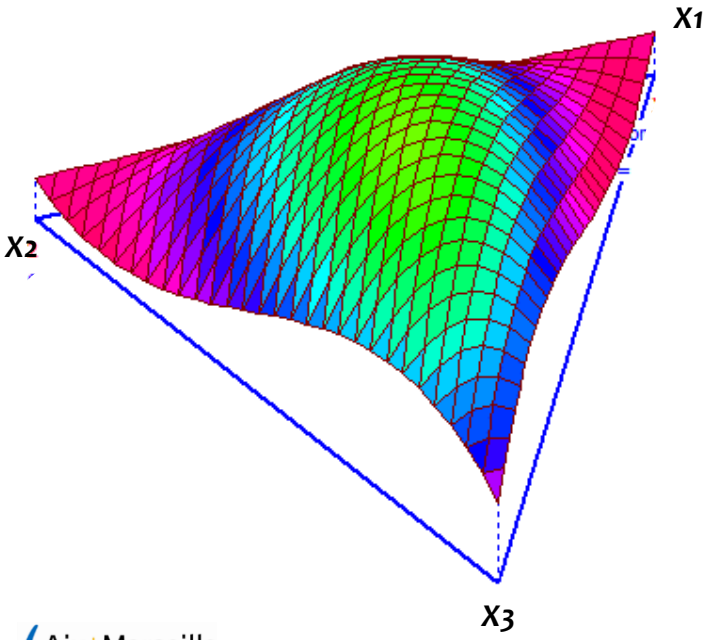


Number of points $N = f(\mathcal{R})$

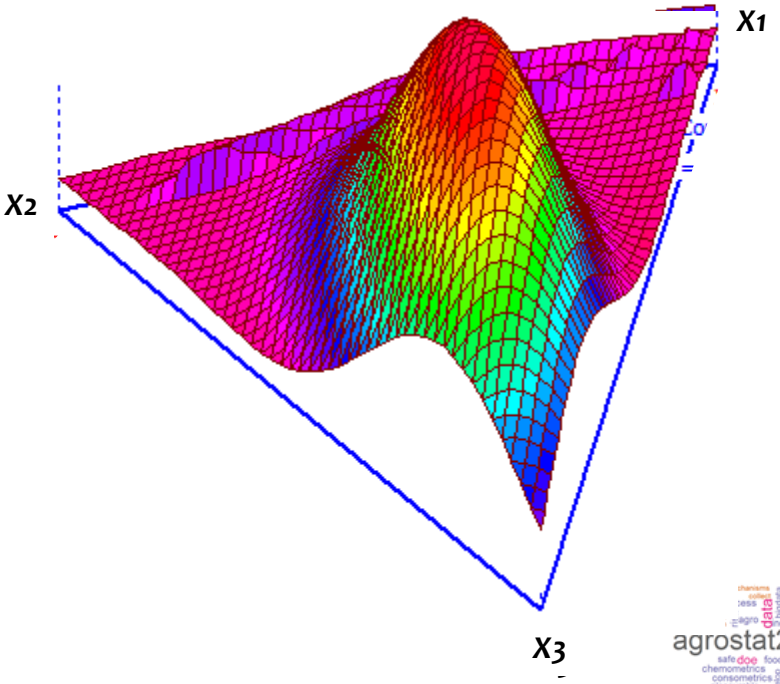
Complex response surface :



Scheffé Simplexe lattice



SbS Design + Kriging



Thank you for your attention !

Any questions

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