Modelling and design of experiments

Chapitre 5: Surface response

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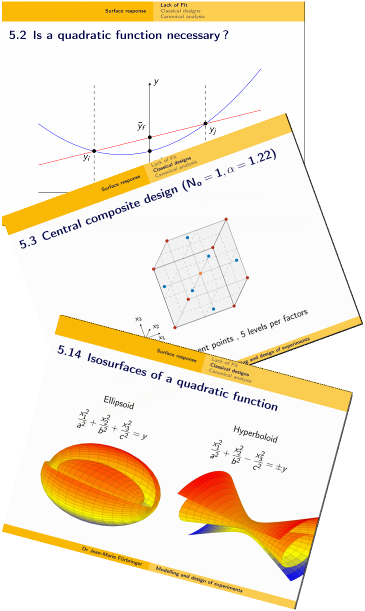
Surface response

1. Lack of fit
2. Classical response surface designs
3. Canonical analysis



5.1 Lack of Fit

5.1.1 Two objectives for performing experiments

1. Quantify the effects of the factors x_i on the response y in a minimal number of experiments to :
   - Select significant factors
   - Perform a Pareto analysis (sort effects by order of importance)

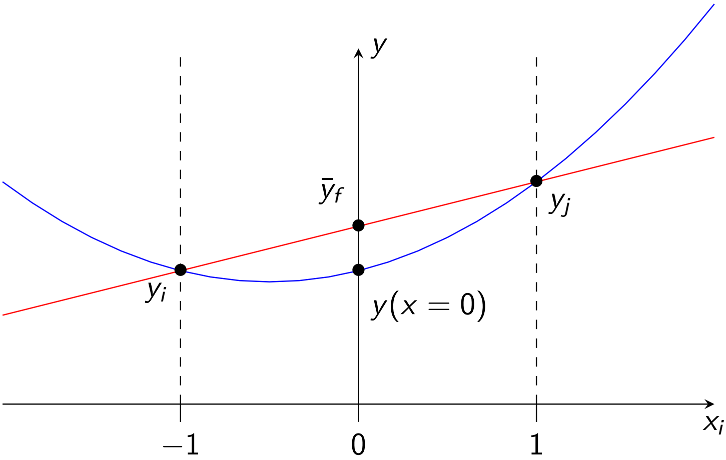
   For this objective a first degree model with or without interactions is sufficient :

$$a_o + \sum_{i=1}^{n} a_i x_i + \sum_{i<j}^{n} a_{ij} x_i x_j$$

2. Determine the combination of the factors that allows us to optimize the response, also with a minimal number of experiments
   For this objective a quadratic model is necessary :

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

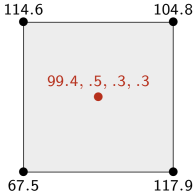
5.1.2 Is a quadratic function necessary ?



5.1.3 Test the curvature with a central point

- An experimental situation with two factors x_1 and x_2, 4 factorial measurements, $y_f(i)$, 4 measurements at the center of the experimental space, $y_c(j)$
- Is the linear model with interactions $y = a_o + a_1 x_1 + a_2 x_2 + a_{12} x_1 x_2$ sufficient ?

Run	Factorial	Center
1	67.5	99.4
2	114.6	99.5
3	117.9	99.3
4	104.8	99.3
$\bar{y}$	101.2	99.4
s^2		0.009
δ	1.83	



Tester $H_o : \alpha_{11} + \alpha_{22} + \cdots = 0$

$$t_o = \frac{\bar{y}_f - \bar{y}_c}{\sqrt{s^2 \left(\frac{1}{n_f} + \frac{1}{n_c}\right)}}$$

if $|t_o| > t_{\alpha/2, n_c - 1}$ then H_o is rejected.

In the present case :
$t_o \approx 27 > t_{0.025,3} \approx 3.18$

5.1.4 With Matlab

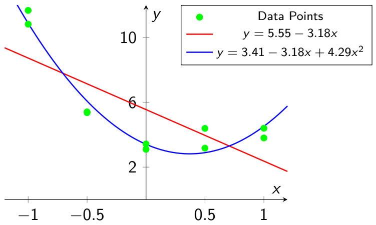
anova(mdl2,'summary')

	SumSq	DF	MeanSq	F	pValue
Total	1613.8	7	230.54		
Model	1607.1	3	535.7	320.36	3.2166e-05
. Linear	701.09	2	350.55	209.63	8.9309e-05
. Nonlinear	906.01	1	906.01	541.81	2.019e-05
Residual	6.6888	4	1.6722		
. Lack of fit	6.6613	1	6.6613	726.68	0.00011202
. Pure error	0.0275	3	0.0091667		

5.1.5 Is there a lack of fit ?

Situation : 10 data points y_i have been acquired for 5 values of x. Is this data better presented by a linear response or a quadratic model ?

	x	y
1	-1	11.67
2	-1	10.82
3	-0.5	5.41
4	-0.5	5.36
5	0	3.10
6	0	3.43
7	0.5	3.17
8	0.5	3.39
9	1	4.40
10	1	3.80



5.1.6 Estimates, residues and sums of squares

i	y	$\bar{y}$	$y-\bar{y}$	$\hat{y}_1$	ϵ_1	$\hat{y}_1-\bar{y}$	$\hat{y}_2$	ϵ_2	$\hat{y}_2-\bar{y}$
1	9.5	10.6	-1.08	9.4	0.12	1.2	10.7	-1.2	-0.12
1	11.7	10.6	1.08	9.4	2.29	1.2	10.7	0.97	-0.12
2	7.9	7.7	0.25	7.7	0.23	-0.02	7.0	0.89	0.64
2	7.4	7.7	-0.25	7.7	-0.28	-0.02	7.0	0.38	0.64
3	3.0	3.5	-0.41	6.0	-2.93	-2.53	4.7	-1.61	-1.21
3	3.9	3.5	0.41	6.0	-2.12	-2.53	4.7	-0.8	-1.21
4	4.9	4.6	0.36	4.3	0.67	0.31	3.6	1.33	0.97
4	4.2	4.6	-0.36	4.3	-0.04	0.31	3.6	0.62	0.97
5	3.0	3.6	-0.6	2.6	0.44	1.03	3.9	-0.88	-0.29
5	4.2	3.6	0.6	2.6	1.63	1.03	3.9	0.31	-0.29
SS	436.8	433.0	3.8	415.0	21.7	18.0	427.2	9.6	5.8

$SS_{PE} = \sum_i (y_{ij} - \bar{y}_i)^2$

$SS_{LOF} = \sum_i (\hat{y}_i - \bar{y}_i)^2$

5.1.7 Differentiate first degree to quadratic model

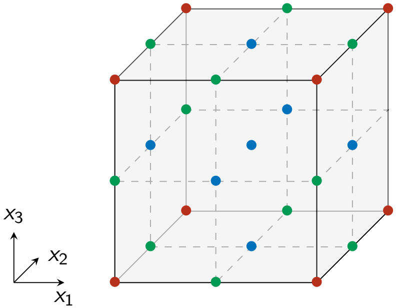
Source	ss	df	ms	F	p
a_o	356.8	1			
Linear	58.3	1	58.3	21.4	0.0017
ϵ_1	21.7	8	2.7		
LoF	18.0	3	6.0	7.9	0.02
Pure error	3.8	5	0.75		

Source	ss	df	ms	F	p
a_o	216.6	1			
Quadratic	210.6	2	105.3	77	0.000017
ϵ_2	9.57	7	1.37		
LoF	5.8	2	2.9	3.9	0.1
Pure error	3.8	5	0.75		

5.2 Classical designs

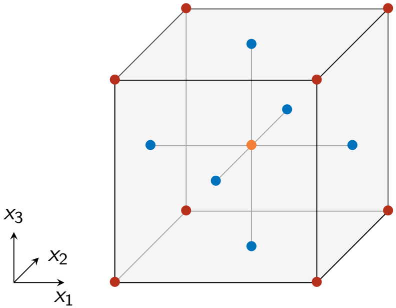
- **Factorial 3^k designs**
- **Composite design**
- **Doehlert design**
- **Box-Behnken**

5.2.1 The 3^k designs



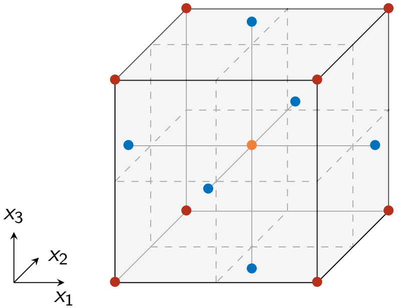
3 factors : 27 measurement points , 3 levels per factor

5.2.2 The central composite design ($\alpha = 1$)



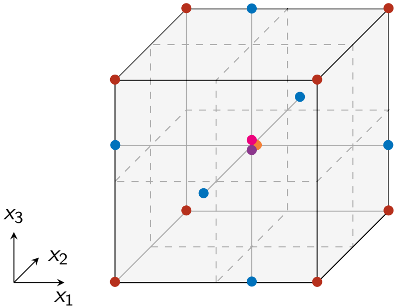
3 factors : 15 measurement points , 3 levels per factors

5.2.3 Central composite design ($N_o = 1, \alpha = 1.22$)



3 factors : 15 measurement points , 5 levels per factors

5.2.4 Central composite design ($N_o = 3, \alpha = 1.353$)



3 factors : 15 measurement points , 3 levels per factors

5.2.5 Optimisation of the radius α

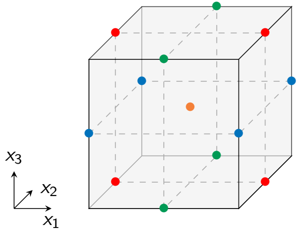
Trade off between *isovariance* per rotation and *pseudo-orthogonality*

- The isovariance per rotation (rotability) : $var_y(x_1, x_2, \ldots) = var_y(\sqrt{x_1 + x_2 + \ldots}$
- The pseudo-orthogonality : property limiting the number of terms in the matrix of dispersion (improve the accuracy of the estimated coefficients).
- Matlab : *E = ccdesign(n)*

Nb of factors (n)	2	3	4	5	5	6	6
Factorial design	22	2^3	2^4	2^{5-1}	2^5	2^{6-1}	2^6
Nb fact exp (2^{n-k})	4	8	16	16	32	32	64
Nbr star pts ($2n$)	4	6	8	10	10	12	12
Nbr central pts (n_o)	1-3	1-3	1-3	1-3	1-3	1-3	1-3
Total ($2^{n-k} + 2n + N_{o)}$	9-11	15-17	25-27	27-29	43-45	45-45	77-79
α si $n_o = 1$	1	1.22	1.41	1.55	1.60	1.72	1.76
α si $n_o = 2$	1.08	1.29	1.48	1.61	1.66	1.78	1.82
α si $n_o = 3$	1.15	1.35	1.55	1.66	1.72	1.83	1.89

5.2.6 Box-Behnken design

$$E = \begin{pmatrix} 0 & -1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \\ -1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & 1 \\ -1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

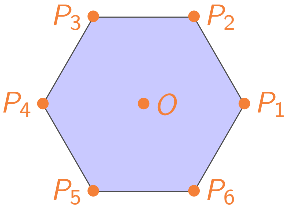


- 3 levels per factor
- No experiments at the vertices
- Isovariant per rotation : 4 ou 7 factors
- Blocking : factorial design 2^2
- Matlab : $E = bbdesign(n)$

Factors	Coefficients	Run
3	10	13
4	15	25
5	21	41
6	28	49

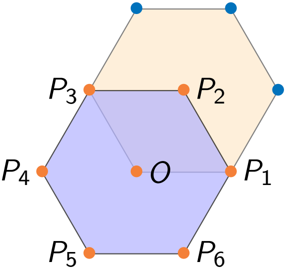
5.2.7 2D Doehlert design

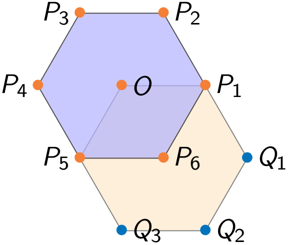
$$E = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -1 & 0 \\ \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{1}{2} & -\frac{\sqrt{3}}{2} \end{pmatrix}$$

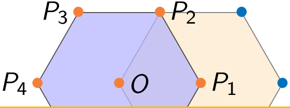


- 2 factors : 7 mesurement points, 3 and 5 levels per factor,
- No experiments at the vertices
- Isovariant per rotation
- Matlab : $E = doehlert(n)$ to download from Moodle

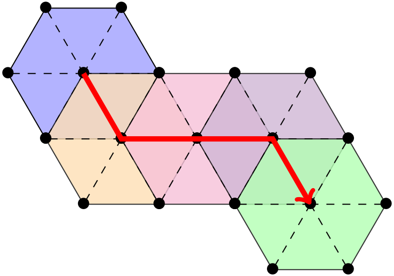
5.2.8 Shift of a 2D Doehlert design





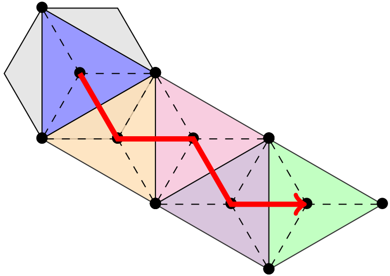


5.2.9 Hexagonal simplex



- Sequential exploration of a domain (7+3+3+3+3=19 exp)

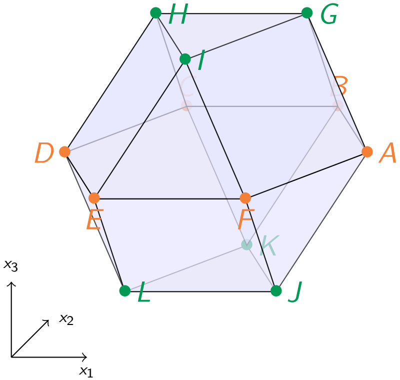
5.2.10 Triangular simplex



- Exploration séquentielle du domaine (3+1+1+1+1=7 exp)

5.2.11 3D Doehlert design

$$E = \begin{pmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 1 & 0 & 0 \\ -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{2}\,\sqrt{3}}{3} \\ \frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{2}\,\sqrt{3}}{3} \\ -\frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{2}\,\sqrt{3}}{3} \\ \frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{2}\,\sqrt{3}}{3} \\ 0 & -\frac{\sqrt{3}}{3} & \frac{\sqrt{2}\,\sqrt{3}}{3} \\ 0 & \frac{\sqrt{3}}{3} & -\frac{\sqrt{2}\,\sqrt{3}}{3} \end{pmatrix}$$



5.2.12 Sequentiality with Doehlert designs

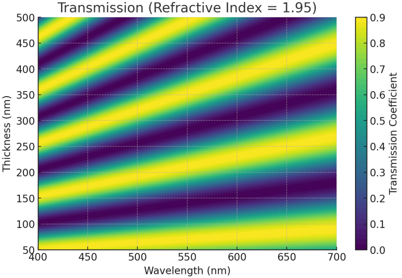
$$E = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 \\
-\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 & 0 \\
\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 & 0 \\
-\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 & 0 \\
\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 & 0 \\
-\frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{2}\sqrt{3}}{3} & 0 & 0 \\
\frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{2}\sqrt{3}}{3} & 0 & 0 \\
-\frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{2}\sqrt{3}}{3} & 0 & 0 \\
\frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{2}\sqrt{3}}{3} & 0 & 0 \\
0 & -\frac{\sqrt{3}}{3} & \frac{\sqrt{2}\sqrt{3}}{3} & 0 & 0 \\
0 & \frac{\sqrt{3}}{3} & -\frac{\sqrt{2}\sqrt{3}}{3} & 0 & 0 \\
-\frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{2}\sqrt{5}}{4} & 0 \\
\frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{6}}{12} & \frac{\sqrt{2}\sqrt{5}}{4} & 0 \\
-\frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{6}}{12} & \frac{\sqrt{2}\sqrt{5}}{4} & 0 \\
\frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{2}\sqrt{5}}{4} & 0 \\
0 & -\frac{\sqrt{3}}{3} & \frac{\sqrt{6}}{12} & \frac{\sqrt{2}\sqrt{5}}{4} & 0 \\
0 & \frac{\sqrt{3}}{3} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{2}\sqrt{5}}{4} & 0 \\
0 & 0 & -\frac{\sqrt{2}\sqrt{3}}{4} & \frac{\sqrt{2}\sqrt{5}}{4} & 0 \\
0 & 0 & \frac{\sqrt{2}\sqrt{3}}{4} & -\frac{\sqrt{2}\sqrt{5}}{4} & 0 \\
-\frac{1}{2} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{10}}{20} & -\frac{\sqrt{3}\sqrt{5}}{5} \\
\frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{6}}{12} & \frac{\sqrt{10}}{20} & \frac{\sqrt{3}\sqrt{5}}{5} \\
-\frac{1}{2} & \frac{\sqrt{3}}{6} & \frac{\sqrt{6}}{12} & \frac{\sqrt{10}}{20} & \frac{\sqrt{3}\sqrt{5}}{5}
\end{pmatrix}$$

5.2.13 Application : light transmission

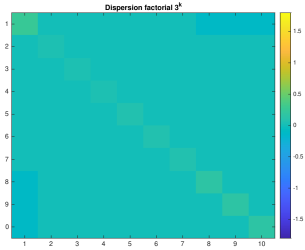
- The transmission or reflection of light by a thin film is a complex phenomenon.
- Based on Snell and Fresnel equations, for a perpendicular non-polarized beam, the transmission coefficient T giving the fraction of intensity which is transmitted is function of the wave length λ, of the refractive index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

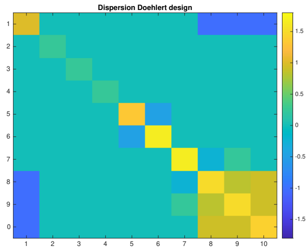
$$T = \left(1 - \left(\frac{n-1}{n+1}\right)^2\right) \sin^2\left(\frac{2\pi nt}{\lambda}\right)$$

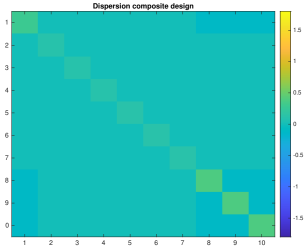
- The objective is to experimentally determine R around the point ($\lambda = 475\ nm(blue), t = 425\ nm, n = 1.95$)

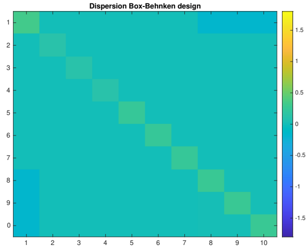


5.2.14 Dispersion matrices



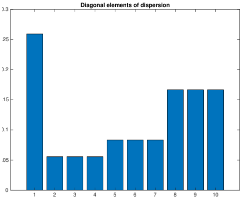




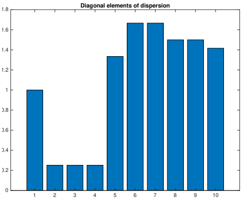


5.2.15 Diagonal elements of dispersion

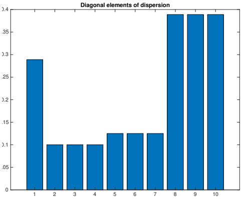
Factorial 2^k



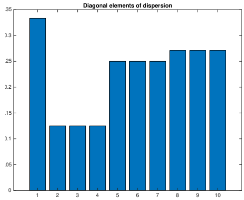
Doehlert



Composite

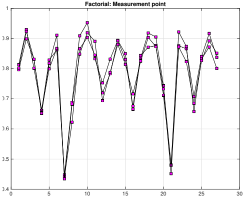


Box-Behnken

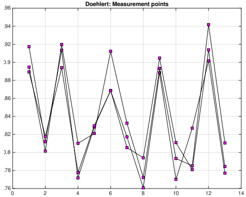


5.2.16 Data points

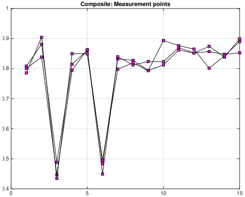
Factorial 2^k



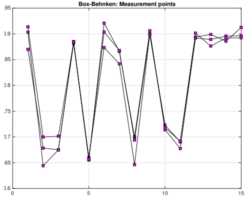
Doehlert



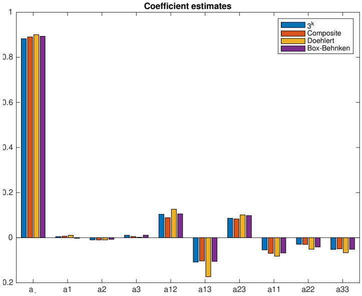
Composite

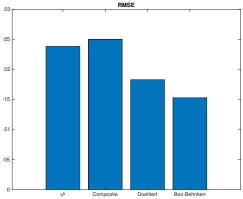


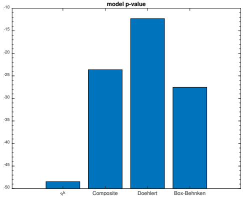
Box-Behnken



5.2.17 Fit

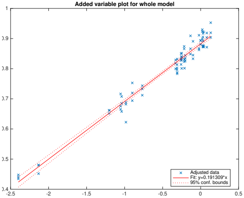

Coefficient estimates
3^k
Composite
Doehlert
Box-Behnken
a1
a2
a3
a12
a13
a23
a11
a22
a33


RMSE
3^k
Composite
Doehlert
Box-Behnken

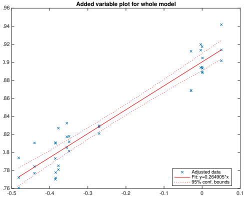

model p-value
3^k
Composite
Doehlert
Box-Behnken

5.2.18 Plot added

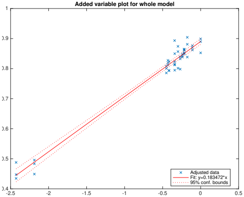
Factorial 2^k



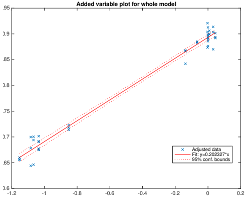
Doehlert



Composite



Box-Behnken



5.3 Canonical analysis

5.3.1 Geometry of the second degree

- The function $a_o + \sum_{i=1}^{n} a_i x_i + \sum_{i \leqslant j}^{n} a_{ij} x_i x_j$ can be written as

$$y = a_o + (x_1, \ldots, x_n) \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} + (x_1, \ldots, x_n) \begin{pmatrix} a_{11} & & \frac{1}{2} a_{1n} \\ & \ddots & \\ \frac{1}{2} a_{1n} & & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

- Equivalent to :

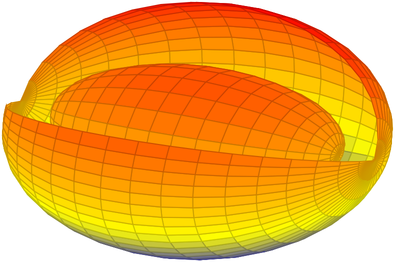
$$y = a_o + \vec{x} \cdot \vec{a} + \vec{x}^T A \vec{x}$$

- The *isosurfaces* of such a function are ellipsoids, or hyperboloids

5.3.2 Isosurfaces of a quadratic function

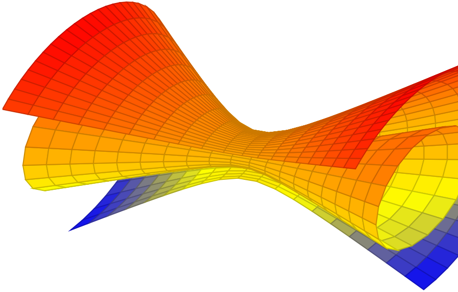
Ellipsoid

$$\frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} + \frac{x_3^2}{c^2} = y$$



Hyperboloid

$$\frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} - \frac{x_3^2}{c^2} = \pm y$$



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 $\nabla y = 0$

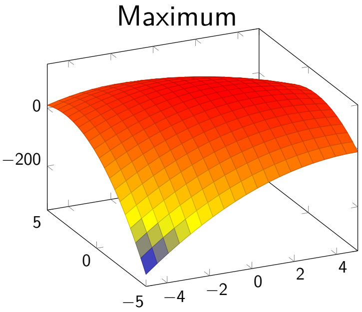
$$
\begin{aligned}
\frac{\partial y}{\partial x_i} &= a_i + a_{1i}x_1 + \ldots + 2a_{ii}x_i + \ldots + a_{in}x_n = 0 \\
0 &= \vec{a} + 2A\vec{x} \\
\vec{x}_s &= -\frac{1}{2}A^{-1}\vec{a} \\
y_s &= a_o + \vec{x}_s \cdot \vec{a} + \vec{x}_s^{\,T} A \vec{x}_s
\end{aligned}
$$

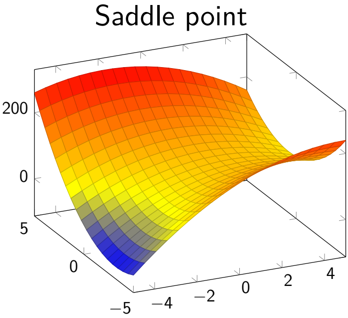
5.4.2 Canonical analysis - main axes

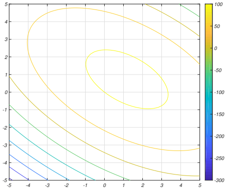
- Main axes are the eigen vectors A, $\tilde{x}_1, \tilde{x}_2, \tilde{x}_3$
- The increase of the function $y = f(\vec{x})$ in the direction corresponding to the main axes is given by the eigen values, $\lambda_1, \lambda_2, \lambda_3$
- In the directions where the eigen values are bigger, the contour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

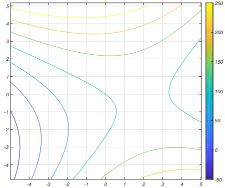
$$y = y_s + \sum_{i=1}^{n} \lambda_i \widetilde{X}_i^2$$

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


Maximum
0
−200
5
0
−5
−4
−2
0
2
4


Saddle point
200
0
5
0
−5
−4
−2
0
2
4



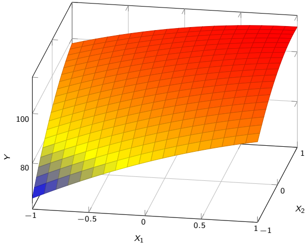


5.4.3 Canonical analysis - example

- Original model
$y = 100 + 10x_1 + 12x_2 - 4x_1x_2 - 3x_1^2 - 5x_2^2$

- Fix point determination

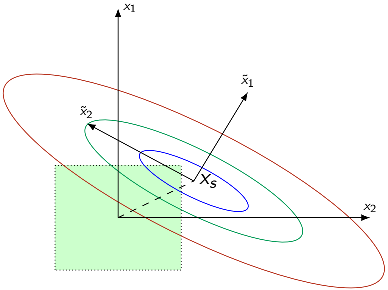
$$A = \begin{pmatrix} -3 & -2 \\ -2 & -5 \end{pmatrix} \quad \vec{a} = \begin{pmatrix} 10 \\ 12 \end{pmatrix} \Rightarrow \vec{x}_s = \begin{pmatrix} 1.18 \\ 0.73 \end{pmatrix}$$



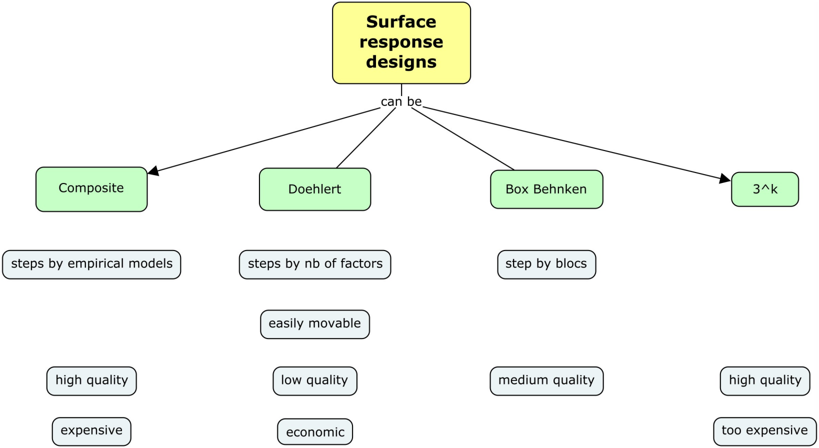
- Eigen values and eigen vectors

$$\begin{cases} \lambda_1 = -6.2 \\ \lambda_2 = -1.8 \end{cases} \quad \text{et} \quad \begin{cases} \tilde{x}_1 = 0.53\hat{x}_1 + 0.85\hat{x}_2 \\ \tilde{x}_2 = -.85\hat{x}_1 + 0.53\hat{x}_2 \end{cases}$$

- Canonical model
$\tilde{y} = 110.3 - 6.2\ \tilde{x}_1^2 - 1.8\ \tilde{x}_2^2$



5.4.4 Surface response designs : pro & cons



5.4.5 Conclusion