Experimental Design and Biostatistics (TAMS38)
Lecture 10 – Response surface

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Response surface

We start by studying a 2^2 design with two observations per combination.

The two factors A and B has low and high level coded as -1 and 1:

A \ B		-1	1
A	-1	$y_{-1,-1,1},\ y_{-1,-1,2}$	$y_{-1,1,1},\ y_{-1,1,2}$
	1	$y_{1,-1,1},\ y_{1,-1,2}$	$y_{1,1,1},\ y_{1,1,2}$

We write the model $Y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ijk}$ as

$$\begin{pmatrix} Y_{-1,-1,1} \\ Y_{-1,1,1} \\ Y_{1,-1,1} \\ Y_{1,1,1} \\ Y_{-1,-1,2} \\ Y_{-1,1,2} \\ Y_{1,-1,2} \\ Y_{1,1,2} \end{pmatrix} = \overset{\begin{matrix} & A & B & AB \end{matrix}}{\underset{\begin{matrix} & x_1 & x_2 & x_1x_2 \end{matrix}}{\begin{pmatrix} 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \end{pmatrix}}} \begin{pmatrix} \mu \\ \tau_1 \\ \beta_1 \\ (\tau\beta)_{11} \end{pmatrix} + \begin{pmatrix} \varepsilon_{-1,-1,1} \\ \varepsilon_{-1,1,1} \\ \varepsilon_{1,-1,1} \\ \varepsilon_{1,1,1} \\ \varepsilon_{-1,-1,2} \\ \varepsilon_{-1,1,2} \\ \varepsilon_{1,-1,2} \\ \varepsilon_{1,1,2} \end{pmatrix} \quad (1)$$

Hence, we have a linear recession model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12}\, x_1 x_2 + \varepsilon \tag{2}$$

Note. Not the same β_1 as in (1).

With matrices we have

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

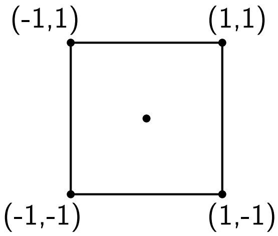
and $\hat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$. This is exactly the same estimators of μ, τ_1, β_1 and $(\tau\beta)_{11}$ as before. (Exercise: Show it!)

In a similar way we will have the models for the 2^k design, where $k \geq 3$.

Assume that both A and B are quantitative factors, e.g., temperature, time, pressure, etc.

We have coded values for the levels as -1 and 1, respectively.

We can now use the model (2) above. Let every x_i vary between -1 to 1 continuously, then will we have a *response surface*.



If we add more observations in the center point, then can we test for quadratic effects, i.e., if we should add the terms x_1^2 and x_2^2 to the model.

We will test for quadratic effects using the mean value for the corner points $\bar{y}_F$ and the mean value for the observations in the center point $\bar{y}_C$.

General case - central points

Above we started with a 2^2 design and constructed a linear regression model with predictors x_1 and x_2 which are -1 and 1.

In the general case for a 2^k design with quantitative factors the linear regression model is given by

$$Y = \beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum_{\{i,j|i<j\}} \beta_{ij} x_i x_j + \varepsilon \tag{3}$$

if we just add the two-way interactions and skip the interactions of higher order.

The interaction terms gives some curvature to the response surface but sometimes it is not enough to explain the surface.

Add second order terms

$$Y = \beta'_0 + \sum_{j=1}^{k} \beta'_j x_j + \sum_{(i,j):i<j} \beta'_{ij} x_i x_j + \sum_{j=1}^{k} \beta'_{jj} x_j^2 + \varepsilon'. \qquad (4)$$

which describes **second-order response surface**.

Note that in the corner observations where x_j is -1 or 1 we adjust $\mathrm{E}(Y)$ with the constant term $\sum_{j=1}^{k} \beta'_{jj}$, but we need more observations to estimate these parameters.

If we also take observations in the center point, where

$$x_1 = \ldots = x_k = 0,$$

then we can estimate σ^2 and test for curvature.

The extra observations in the center will not change the estimators of the main and interaction effects for the original 2^k design.

To test curvature we will compare

- the mean value of the n_F observations in the corners, $\bar{y}_F$, with
- the mean value of the n_C observations in the center point, $\bar{y}_C$.

The expectations for these means are

$$E(\bar{Y}_F) = \beta_0' + \sum_{j=1}^{k} \beta_{jj}' \quad \text{and} \quad E(\bar{Y}_C) = \beta_0'$$

while both of them are β_0 in the smaller model (3).

If the mean values $E(\bar{Y}_F)$ and $E(\bar{Y}_C)$ **not** are equal this indicates that the second order terms are needed, i.e., that curvature exists.

Example 1 – 2^1 design

Two observations $(-1, y_{-1})$ and $(1, y_1)$. If linear, i.e., no curvature, then $y_0 = \frac{y_{-1}+y_1}{2}$. But, if curvature then are y_0 and $\frac{y_{-1}+y_1}{2}$ not equal.

Figure: 2^1-factorial design

Example 2 – 2^2 design

For the factorial design we have $n_F = 2^2 = 4$ observations in the corners and the model

$$Y_{ij} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ij},$$

and given as a linear regression model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon,$$

where $\beta_0 = \mu$.

In this model $\mathrm{E}(Y) = \beta_0$, when $x_1 = x_2 = 0$.

Hence,

$$\hat{\beta}_0 = \hat{\mu} = \bar{y}_{..} = \bar{y}_F \leftarrow \text{ new notation},$$

which is $\bar{Y}_F \sim N\left(\mu, \frac{\sigma^2}{n_F}\right)$.

In the center point we have $y_{C1}, \ldots, y_{Cn_C}$, where

$$Y_{Ck} \sim N(\underbrace{\mu + \Delta}_{=\mu_C}, \sigma^2).$$

Furthermore,

$$\hat{\mu}_C = \bar{Y}_C \sim N\left(\mu_C, \frac{\sigma^2}{n_C}\right).$$

We want to compare $\hat{\mu} = \bar{y}_F$ and $\hat{\mu}_C = \bar{y}_C$..

$$\bar{Y}_F - \bar{Y}_C \sim N\left(\mu - \mu_C, \sigma^2\left(\frac{1}{n_F} + \frac{1}{n_C}\right)\right).$$

If $\mu = \mu_C$, i.e., no curvature, then

$$\frac{\bar{Y}_F - \bar{Y}_C - 0}{\sigma\sqrt{\frac{1}{n_F} + \frac{1}{n_C}}} \sim N(0, 1)$$

and

$$\frac{\left(\bar{Y}_F - \bar{Y}_C\right)^2}{\sigma^2\left(\frac{1}{n_F} + \frac{1}{n_C}\right)} \sim \chi^2(1).$$

Test for curvature

If we have n_F corner points, i.e., observations for the 2^k or 2^{k-p} design, and n_C observations in the center point then define

$$SS_{PQ} = \frac{(\bar{y}_F - \bar{y}_C)^2}{\frac{1}{n_F} + \frac{1}{n_C}} = \frac{n_F n_C (\bar{y}_F - \bar{y}_C)^2}{n_C + n_F},$$

($PQ=$ pure quadratic).

a) If we have one observation per combination then curvature is tested with the test statistic

$$v_{PQ} = \frac{SS_{PQ}}{s^2} = \frac{SS_{PQ}/1}{(n_C - 1)s^2/(n_C - 1)},$$

where $s^2 = \frac{1}{n_C - 1} \sum_{k=1}^{n_C} (y_{Ck} - \bar{y}_C)^2$, i.e., the sample variance for the center observations.

The hypothesis

$$H_0\text{: "no curvature" , i.e., } \Delta = 0$$

is rejected for large values of v_{PQ}.

If H_0 is true, then $V_{PQ} \sim F(1, n_C - 1)$.

b) For the general case (more than one observation per combination), we have

$$v_{PQ} = \frac{SS_{PQ}}{SS_E/df_E}$$

and $V_{PQ} \sim F(1, df_E)$ if H_0 is true.

To estimate all the parameters for the model with curvature we need more observations.

Example 3

Let Minitab generate a 2^2-design with five observations in the center point.

Do your experiment according to the proposed design and add the response values (y).

Minitab - Untitled - [Worksheet 1 ***]

File Edit Data Calc Stat Graph Editor Tools Window Help

↓	C1	C2	C3	C4	C5	C6	C7
	StdOrder	RunOrder	CenterPt	Blocks	A	B	
1	2	1	1	1	1	-1	36
2	5	2	0	1	0	0	32
3	7	3	0	1	0	0	34
4	9	4	0	1	0	0	36
5	1	5	1	1	-1	-1	27
6	6	6	0	1	0	0	31
7	3	7	1	1	-1	1	33
8	8	8	0	1	0	0	30
9	4	9	1	1	1	1	41
10							

We have

$$\bar{y}_F = \frac{1}{4}(27 + 41 + 33 + 36) = 34.25,$$

$$\bar{y}_C = \frac{1}{5}(32 + 34 + 36 + 31 + 30) = 32.6,$$

$$\hat{\Delta} = \bar{y}_C - \bar{y}_F = -1.65$$

and $s = 2.408$ with $df = 4$, where s is the sample standard deviation for the center points.

$$SS_{PQ} = \frac{(\bar{y}_C - \bar{y}_F)^2}{\frac{1}{5} + \frac{1}{4}} = 6.05,$$

$$v_{PQ} = \frac{SS_{PQ}/1}{s^2} = 1.04 < 7.71 = F_{0.95}(1, 4).$$

Hence, the curvature is not significant.

STAT-DOA-Factorial-Create Factorial Design

```
MTB > Name C1 "StdOrder" C2 "RunOrder" C3 "CenterPt"
                                  C4 "Blocks" C5 "A" C6 "B"
MTB > FFDesign 2 4;
SUBC>   CPBlocks 5;
SUBC>   CTPT 'CenterPt';
SUBC>   Randomize;
SUBC>   SOrder 'StdOrder' 'RunOrder';
SUBC>   Alias 2;
SUBC>   XMatrix 'A' 'B'.

Full Factorial Design

Factors:   2   Base Design:         2, 4
Runs:      9   Replicates:             1
Blocks:    1   Center pts (total):     5

All terms are free from aliasing.
```

```
MTB > FFactorial C7 = C5 C6 C5*C6;
SUBC>   Design C5 C6 C4;
SUBC>   Order C1;
SUBC>   InUnit 1;
SUBC>   Levels -1 1 -1 1;
SUBC>   CTPT C3;
SUBC>   FitC;
SUBC>   Brief 2;
SUBC>   Alias.

Factorial Fit: C7 versus A, B

Estimated Effects and Coefficients for C7 (coded units)

Term       Effect    Coef  SE Coef      T      P
Constant           34.250    1.204  28.44  0.000
A           8.500   4.250    1.204   3.53  0.024
B           5.500   2.750    1.204   2.28  0.084
A*B        -0.500  -0.250    1.204  -0.21  0.846
Ct Pt              -1.650    1.616  -1.02  0.365

S = 2.40832      PRESS = *
R-Sq = 82.42%   R-Sq(pred) = *%   R-Sq(adj) = 64.85%
```

Analysis of Variance for C7 (coded units)

Source	DF	Seq SS	Adj SS	Adj MS	F	P
Main Effects	2	102.500	102.500	51.2500	8.84	0.034
2-Way Interactions	1	0.250	0.250	0.2500	0.04	0.846
Curvature	1	6.050	6.050	6.0500	1.04	0.365
Residual Error	4	23.200	23.200	5.8000		
Pure Error	4	23.200	23.200	5.8000		
Total	8	132.000				

How to choose more observations?

When we want to estimate the model including curvature we need more observations. The question is how to choose these.

For a 2^2 design, we have the model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \varepsilon,$$

where x_1 and x_2 are coded for the quantitative factors.

We have six parameters and we need at least six observations to estimate all these.

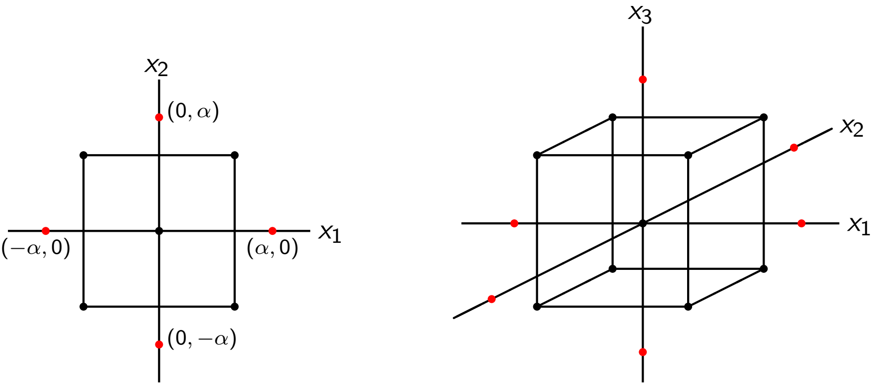
Extended designs

There are several ways to extend design so that one can estimate a second-order model (see book, Section 11.4).

Central composite design (CCD) is the manner and may be used to estimate the parameters of a quadratic surface (second-order model).

If we let n_C, i.e., number of measurements in the central point, fulfill $1 \leq n_C \leq 5$, but obviously it is good to do a few more measurements there.

Central composite designs (CCD)



Central composite designs (CCD) for $k = 2$ and $k = 3$.

It is important for the second-order model to provide good predictions throughout the region of interest
$\Rightarrow$ require reasonably consistent and stable variance.

The second-order response surface design should be *rotatable*, i.e., same variance for all points with same distance from the center.

A CCD is made rotatable by a good choice of α.

The value of α for rotability depends on the number of points in the factorial portion of the design, in fact $\alpha = n_F^{1/4}$ yields a rotatable CCD.

For a spherical region of interest, the best choice of α from a prediction variance viewpoint for the CCD is to set $\alpha = \sqrt{k}$.
$\Rightarrow$ This design, called *spherical CCD*, puts all the factorial and axial design points on the surface of a sphere of radius $\sqrt{k}$.

If you have enough data points, you can also take the third-order terms into the model. Then, one does a polynomial approximation of a surface.

It is important to remember that such approximations works great **locally**. For a large area with sparse points should be cautious and try to verify their results, for example, by making several new measurements in the optimal point that one obtained.

Often one limits itself to an interesting area before making extended design, see course book Chapter 11.2, The method of steepest ascent, as well as the following example.

Example 4 – Response surface

In a study one wants to find the best combination of time (t) and temperature (T) which produce the maximum amount of a specific substancee in a chemical process.

We think that the best combination is around the time $t = 75$ minutes and temperature $T = 130^\circ$C.

Let the time vary from 70 to 80 minutes and the temperature from 127.5 to 132.5°C as in the Table 1. We have coded our variables as

$$x_1 = \frac{t - 75 \text{ minutes}}{5 \text{ minutes}}, \quad x_2 = \frac{T - 130^\circ\text{C}}{2.5^\circ\text{C}}.$$

Table 1: Result from the first design with three center points

	Variables in original units		Variables in coded units		Respons: amount
run	time	temp	x_1	x_2	y
1	70	127.5	-1	-1	54.3
2	80	127.5	$+1$	-1	60.3
3	70	132.5	-1	$+1$	64.6
4	80	132.5	$+1$	$+1$	68.0
5	75	130.0	0	0	60.3
6	75	130.0	0	0	64.3
7	75	130.0	0	0	62.3

We will use a 2^2 factorial design with three center points.

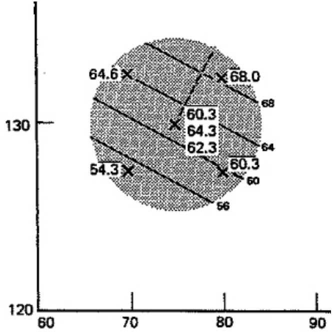


Figure 1.

The design is called a *first-order design* and is good for testing first order polynomial,

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon.$$

We use Minitab command: **Stat/DOE/Factorial/ Create Factorial Design...**

```
MTB > Name C1 "StdOrder" C2 "RunOrder" C3 "CenterPt"
                                   C4 "Blocks" C5 "A" C6 "B"
MTB > FFDesign 2 4;
SUBC>   CPBlocks 3;
SUBC>   CTPT 'CenterPt';
SUBC>   Randomize;
SUBC>   SOrder 'StdOrder' 'RunOrder';
SUBC>   Alias 2;
SUBC>   XMatrix 'A' 'B'.
```

We add the observations y in column c7 (Y).

	C1	C2	C3	C4	C5	C6	C7
	StdOrder	**RunOrder**	**CenterPt**	**Blocks**	**A**	**B**	**Y**
1	1	1	1	1	-1	-1	54,3
2	4	2	1	1	1	1	68,0
3	6	3	0	1	0	0	60,3
4	2	4	1	1	1	-1	60,3
5	3	5	1	1	-1	1	64,6
6	5	6	0	1	0	0	64,3
7	7	7	0	1	0	0	62,3

Analyzing according to a complete model of factorial design with special expectation of the center points.

Stat/DOE/Factorial/Analyze Factorial Design...

```
MTB > FFactorial 'Y' = C5 C6 C5*C6;
SUBC>   Design C5 C6 C4;
SUBC>   Order C1;
SUBC>   InUnit 1;
SUBC>   Levels -1 1 -1 1;
SUBC>   CTPT C3;
SUBC>   FitC;
SUBC>   Brief 2;
SUBC>   Alias.
```

Factorial Fit: Y versus A; B

Estimated Effects and Coefficients for Y (coded units)

Term	Effect	Coef	SE Coef	T	P
Constant		61,8000	1,000	61,80	0,000
A	4,7000	2,3500	1,000	2,35	0,143
B	9,0000	4,5000	1,000	4,50	0,046
A*B	-1,3000	-0,6500	1,000	-0,65	0,582
Ct Pt		0,5000	1,528	0,33	0,775

S = 2 PRESS = *
R-Sq = 92,93% R-Sq(pred) = *% R-Sq(adj) = 78,80%

Analysis of Variance for Y (coded units)

Source	DF	Seq SS	Adj SS	Adj MS	F	P
Main Effects	2	103,090	103,090	51,5450	12,89	0,072
2-Way Interactions	1	1,690	1,690	1,6900	0,42	0,582
Curvature	1	0,429	0,429	0,4286	0,11	0,775
Residual Error	2	8,000	8,000	4,0000		
Pure Error	2	8,000	8,000	4,0000		
Total	6	113,209				

1. $v_{AB} = \dfrac{SS_{AB}/1}{SS_E/2} = 0.42$ with $P = 0.582$, i.e. interaction seems to be negligible.
2. $v_{PQ} = \dfrac{SS_{PQ}/1}{SS_E/2} = 0.11$ with $P = 0.775$, i.e. curvature seems to be negligible.

To emphasize that we change the response surface we change the labels and let $A \to x_1$ and $B \to x_2$.

From 1. and 2. above we do analysis according to the linear model with **Stat/Regression/Regression...**

Regression Analysis: Y versus x1; x2

```
The regression equation is
Y = 62,0 + 2,35 x1 + 4,50 x2

Predictor      Coef  SE Coef       T      P
Constant    62,0143   0,6011  103,16  0,000
x1           2,3500   0,7952    2,96  0,042
x2           4,5000   0,7952    5,66  0,005

S = 1,59049   R-Sq = 91,1%   R-Sq(adj) = 86,6%

Analysis of Variance

Source          DF       SS      MS      F      P
Regression       2  103,090  51,545  20,38  0,008
Residual Error   4   10,119   2,530
Total            6  113,209
```

Observe that we obtain the same coefficients of A and B as in the previous analysis.

Note. Pure error is obtained by calculating s_i^2 for points with repeated observations (for us the center points) and pool them together in the usual manner to an error sum of squares.

We now have an approximately linear relation

$$y = 62.01 + 2.35x_1 + 4.50x_2.$$

We now want to find the steepest ascent.

Suppose that we are in (x_{01}, x_{02}) and should move to (x_{11}, x_{12}). The distance between these points is

$$r = \sqrt{(x_{11} - x_{01})^2 + (x_{12} - x_{02})^2}.$$

We want to move in a direction so the change in the response y is maximal. We have

$$y_0 = 62.01 + 2.35x_{01} + 4.50x_{02},$$
$$y_1 = 62.01 + 2.35x_{11} + 4.50x_{12}.$$

Furthermore,

$$\begin{aligned} y_1 - y_0 &= 2.35(x_{11} - x_{01}) + 4.50(x_{12} - x_{02}) \quad \text{"scalar product"} \\ &\leq \left[(2.35^2 + 4.50^2)((x_{11} - x_{01})^2 + (x_{12} - x_{02})^2)\right]^{1/2} \\ &\qquad\qquad\qquad\qquad\qquad\qquad \text{"Cauchy-Schwarz-ineq.} \\ &= \sqrt{2.35^2 + 4.50^2} \end{aligned}$$

wih equality when $x_{11} - x_{01} = c \cdot 2.35$ and $x_{12} - x_{02} = c \cdot 4.50$.

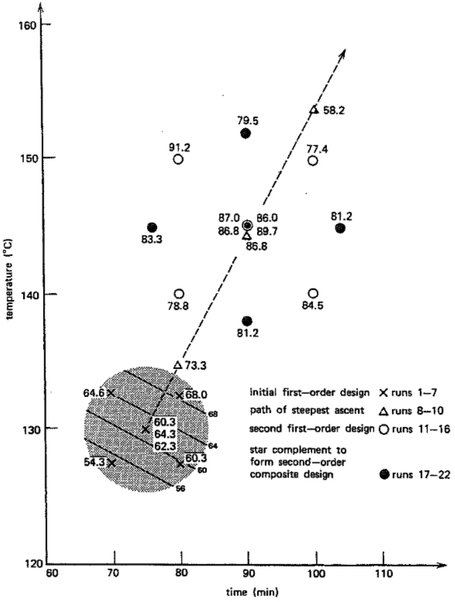
Choose $c = \dfrac{1}{2.35}$.

If x_1 increase with 1 then increase x_2 with $\dfrac{4.50}{2.35} \approx 1.91$.

Start in the center point (0,0) with $y_0 = 62.01$ and take a step in the steepest ascent, se Figure 2 and Table 2.

Table 2: Path of steepest ascent.

Coded variables		Time (min)	Temp (°C)		
x_1	x_2	t	T	run	observation
0	0	75	130.0	5,6,7	62.3 (mean)
1	1.91	80	134.8	8	73.3
2	3.83	85	139.6		
3	5.74	90	144.4	10	86.8
4	7.66	95	149.1		
5	9.57	100	153.9	9	58.2


160
150
140
130
120
60
70
80
90
100
110
time (min)
temperature (°C)
58.2
79.5
91.2
77.4
87.0
86.0
86.8
89.7
86.8
81.2
83.3
78.8
84.5
81.2
73.3
64.6
68.0
60.3
64.3
62.3
54.3
60.3
68
64
60
56
initial first—order design × runs 1—7
path of steepest ascent △ runs 8—10
second first—order design ○ runs 11—16
star complement to
form second—order
composite design ● runs 17—22

Figur 2.

When a new step doesn't give a better value, we stop and try to fit a new response surface with a new factorial design.

Table 3: Result from the second design with two center points

	Variables in original units		Variables in coded units		Response: amount
run	tid	temp	x_1	x_2	y
11	80	140	-1	-1	78.8
12	100	140	$+1$	-1	84.5
13	80	150	-1	$+1$	91.2
14	100	150	$+1$	$+1$	77.4
15	90	145	0	0	89.7
16	90	145	0	0	86.8

Factorial Fit: Y versus A; B

Estimated Effects and Coefficients for Y (coded units)

Term	Effect	Coef	SE Coef	T	P
Constant		82,975	1,025	80,93	0,008
A	-4,050	-2,025	1,025	-1,98	0,298
B	2,650	1,325	1,025	1,29	0,419
A*B	-9,750	-4,875	1,025	-4,75	0,132
Ct Pt		5,275	1,776	2,97	0,207

S = 2,05061 PRESS = *
R-Sq = 97,37% R-Sq(pred) = *% R-Sq(adj) = 86,84%

Analysis of Variance for Y (coded units)

Source	DF	Seq SS	Adj SS	Adj MS	F	P
Main Effects	2	23,425	23,425	11,713	2,79	0,390
2-Way Interactions	1	95,062	95,062	95,062	22,61	0,132
Curvature	1	37,101	37,101	37,101	8,82	0,207
Residual Error	1	4,205	4,205	4,205		
Pure Error	1	4,205	4,205	4,205		
Total	5	159,793				

$P_{AB} = 0.132$ and $P_{PQ} = 0.2067$ indicates that we have some small curvature and interaction, but very few degrees of freedom for the SS_E.

We extend the design to a spherical CCD.

Table 4: Resultat from the extended design

	Variables in original units		Variables in coded units		Response: amount
run	tid	temp	x_1	x_2	y
11	80	140	-1	-1	78.8
12	100	140	$+1$	-1	84.5
13	80	150	-1	$+1$	91.2
14	100	150	$+1$	$+1$	77.4
15	90	145	0	0	89.7
16	90	145	0	0	86.8
Resultat from the second design with extra observations					
17	76	145	$-\sqrt{2}$	0	83.3
18	104	145	$+\sqrt{2}$	0	81.2
19	90	138	0	$-\sqrt{2}$	81.2
20	90	152	0	$+\sqrt{2}$	79.5
21	90	145	0	0	87.0
22	90	145	0	0	86.0

We add the observations to Minitab.

	C1	C2	C3	C4	C5	C6
	x1	x2	x1*x2	x1**2	x2**2	Y
1	-1,00000	-1,00000	1	1	1	78,8
2	0,00000	0,00000	0	0	0	89,7
3	0,00000	0,00000	0	0	0	86,8
4	1,00000	1,00000	1	1	1	77,4
5	-1,00000	1,00000	-1	1	1	91,2
6	1,00000	-1,00000	-1	1	1	84,5
7	-1,41421	0,00000	0	2	0	83,3
8	1,41421	0,00000	0	2	0	81,2
9	0,00000	-1,41421	0	0	2	81,2
10	0,00000	1,41421	0	0	2	79,5
11	0,00000	0,00000	0	0	0	87,0
12	0,00000	0,00000	0	0	0	86,0

Now we can fit the second order polynomial with **STAT/ Regression/Regression...**.

```
The regression equation is
Y = 87,4 - 1,38 x1 + 0,362 x2 - 4,87 x1*x2 - 2,14 x1**2 - 3,09 x2**2

Predictor      Coef  SE Coef      T      P
Constant     87,375    1,002  87,22  0,000
x1          -1,3837   0,7084  -1,95  0,099
x2           0,3620   0,7084   0,51  0,628
x1*x2        -4,875    1,002  -4,87  0,003
x1**2       -2,1437   0,7920  -2,71  0,035
x2**2       -3,0937   0,7920  -3,91  0,008

S = 2,00365   R-Sq = 88,7%   R-Sq(adj) = 79,2%

Analysis of Variance
Source          DF       SS      MS     F      P
Regression       5  188,189  37,638  9,38  0,008
Residual Error   6   24,088   4,015
Total           11  212,277
```

We now have

$$y = 87.375 - 1.3837x_1 + 0.3620x_2 - 4.875x_1x_2 - 2.1437x_1^2 - 3.0937x_2^2,$$

which we can be maximized by completing to squares

$$\begin{aligned}
y &= 87.375 - 2.1437\,\left(0.6455\,x_1 - 0.1689\,x_2 + 2.2741\,x_1x_2 + x_1^2 + 1.4432\,x_2^2\right) \\
&= 87.375 - 2.1437\left[\left(x_1 + \frac{0.6455}{2} + \frac{2.2741}{2}\,x_2\right)^2 - \left(\frac{0.6455}{2}\right)^2\right. \\
&\qquad \left. + \left(\frac{2.2741}{2}\right)^2\,x_2^2 - 2\,\frac{0.6455}{2}\,\frac{2.2741}{2}\,x_2 - 0.1689\,x_2 + 1.4432\,x_2^2\right] \\
&= 87.375 - 2.1437\,\left[(x_1 + 0.3228 + 1.1371\,x_2)^2 - 0.1042\right. \\
&\qquad \left. + 0.1503\,x_2^2 - 0.9029\,x_2\right]
\end{aligned}$$

$$
\begin{aligned}
&= 87.375 - 2.1437 \left[(x_1 + 0.3228 + 1.1371\, x_2)^2 - 0.1042 \right. \\
&\qquad \left. + 0.1503 \left(x_2 - \frac{0.9029}{2 \cdot 0.1503} \right)^2 - \frac{0.9029^2}{4 \cdot 0.1503} \right] \\
&= 87.375 - 2.1437 \left[(x_1 + 0.3228 + 1.1371\, x_2)^2 \right. \\
&\qquad \left. + 0.1503 \, (x_2 - 3.00)^2 - 1.4602 \right] \leq \underline{\underline{90.505}},
\end{aligned}
$$

with equality for $x_2 = 3.00$ and $x_1 = -0.3228 - 1.1371\, x_2$.

Hence, optimum is

$$
\begin{aligned}
x_1 &= -3.74, \\
x_2 &= 3.00,
\end{aligned}
$$

which is not in the studied region... ((i) new design? (ii) outlier?)

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