Response Surface Designs

A response variable Y depends on several explanatory variables. The goal is to optimize the value of Y.

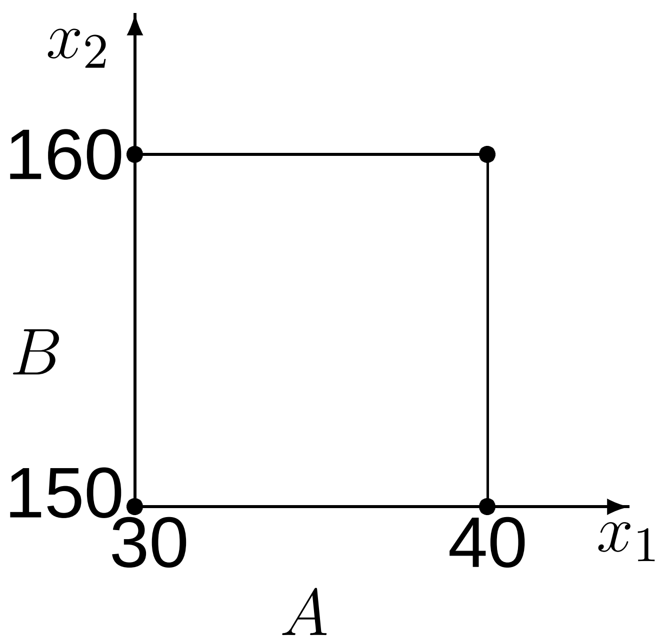
$$Y = f(x_1, x_2) + \epsilon, \qquad \text{function f is unknown.}$$

$f(x_1, x_2)$ is called response surface.

Maximal yield of a chemical process

The yield Y of a chemical process depends on reaction time (A) and temperature (B). Current conditions are 35 min. and 155°C.

2^2-factorial:



$$x_1 = \frac{\text{time} - 35}{5}$$

$$x_2 = \frac{\text{temp} - 155}{5}$$

First-order Model

run	A	B	x_1	x_2	y
1	30	150	–1	–1	39.3
2	40	150	+1	–1	40.9
3	30	160	–1	+1	40.0
4	40	160	+1	+1	41.5

First-order model: $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$

R Output

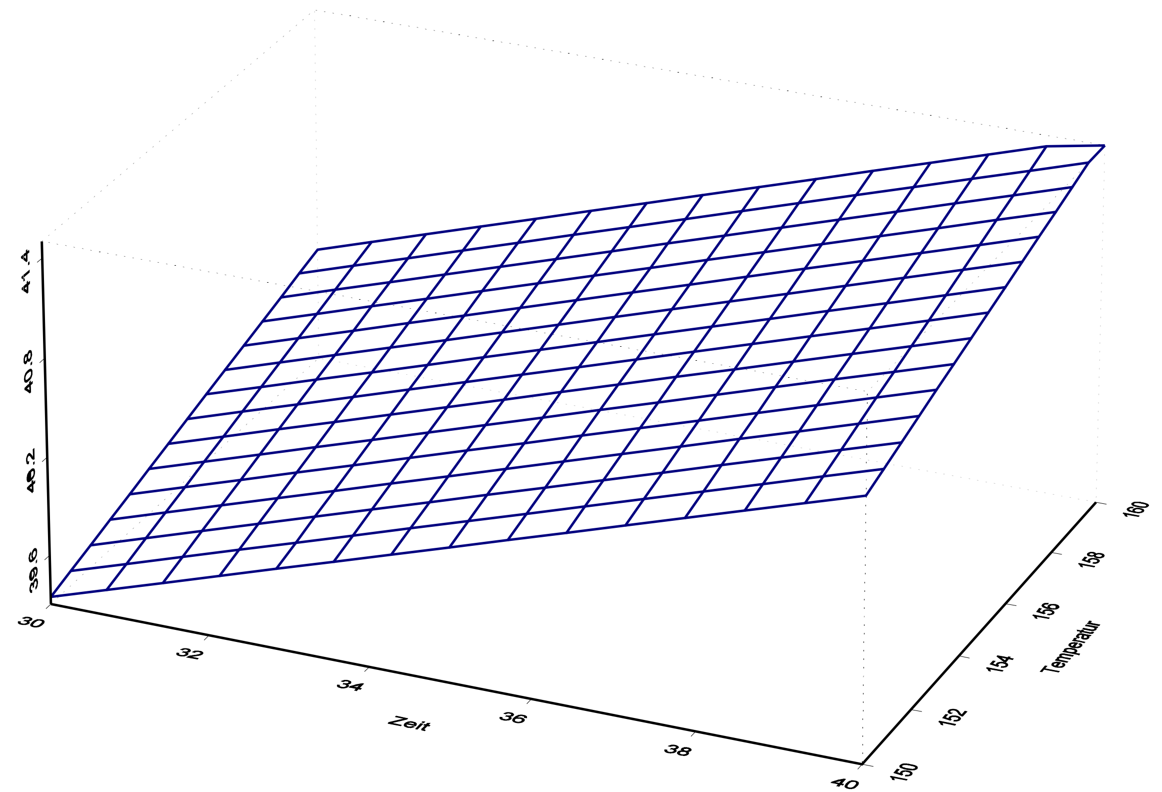
```
> summary(mod1)
Call: lm(formula = y ~ x1 + x2)

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   40.425      0.025    1617 0.000394 ***
x1             0.775      0.025      31 0.020529 *
x2             0.325      0.025      13 0.048875 *

Residual standard error: 0.05 on 1 df
Multiple R-squared: 0.9991, Adj R-squared: 0.9973
F-statistic: 565 on 2 and 1 DF, p-value: 0.02974
```

First order response

$$\hat{y} = 40.425 + 0.775x_1 + 0.325x_2$$



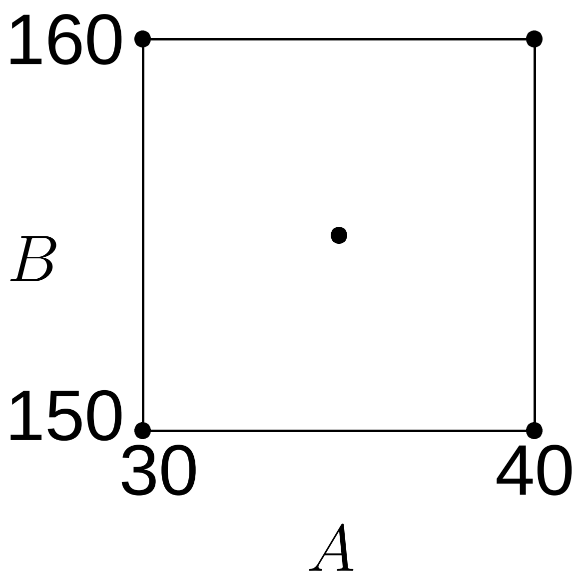
Model with interaction

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

$\hat{\beta}_{12} = -0.025$, perfect fit, no estimation of σ.

- Additional runs are necessary to estimate the experimental error and test the interaction effect.
- We add five observations at the center to get an independent estimation of σ and check the fit of the first-order model or a curvature.

Factorial with center points



A	B	x_1	x_2	y
35	155	0	0	40.3
35	155	0	0	40.5
35	155	0	0	40.7
35	155	0	0	40.2
35	155	0	0	40.6

Checking Curvature and Interaction

- Second-order model
  $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \epsilon$
- Estimation of curvature: mean in factorial – mean at center $= \bar{y}_f - \bar{y}_c = 40.425 - 40.46 = -0.035.$
  $\bar{y}_f - \bar{y}_c$ is an estimate for $\beta_{11} + \beta_{22}$
- Estimation of σ^2:

$$MS_{res} = \frac{\sum^5 (y_i - \bar{y}_c)^2}{4} = 0.043$$

- Can construct confidence intervals for β_{12} and $\beta_{11} + \beta_{22}$. First-order model is adequate.

Method of steepest ascent

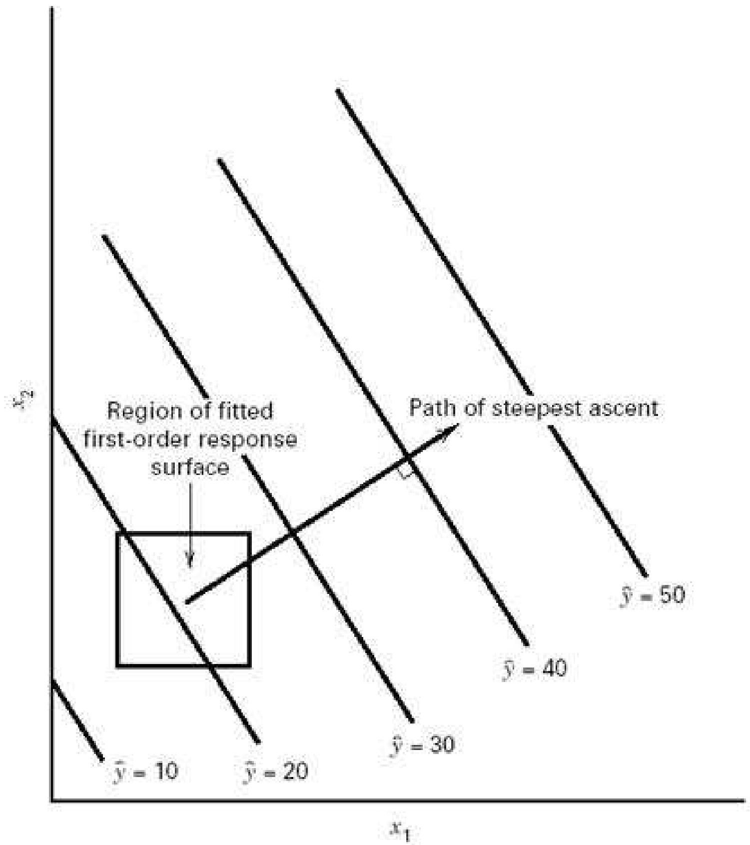


Figure 11-4 First-order response surface and path of steepest ascent.

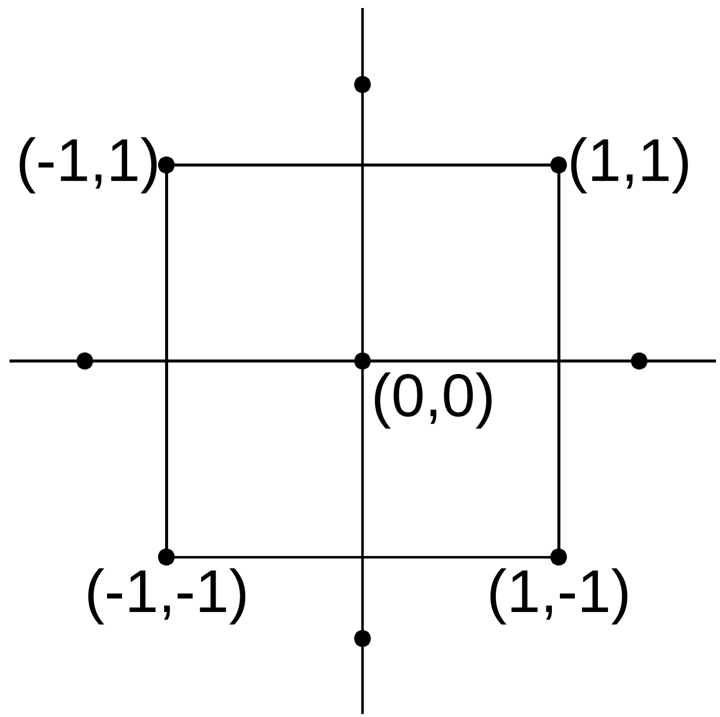
Example: $\hat{y} = 40.44 + 0.775x_1 + 0.325x_2$

contour lines $x_2 = -\frac{0.775}{0.325}x_1 + c$,
direction of steepest ascent: $\frac{0.325}{0.775} = 0.42$
additional observations:

A	B	x_1	x_2	y
35	155	0	0	
40	157.1	1	0.42	40.5
45	159.2	2	0.84	51.3
50	161.3	3	1.26	59.6
55	163.4	4	1.68	67.1
60	165.5	5	2.10	63.6
65	167.6	6	2.52	60.7

Second-order model around (55,163)

Central Composite Design



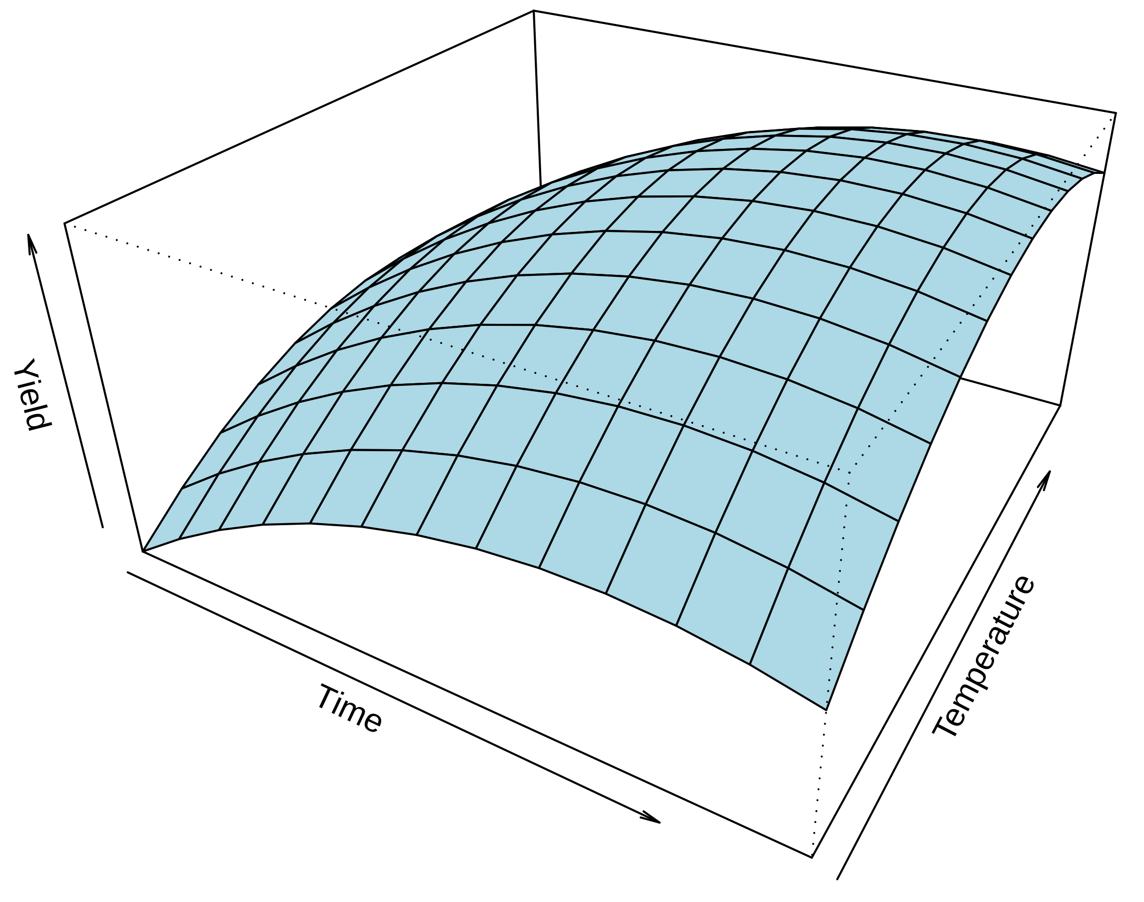
Data

Time	Temperature	x_1	x_2	Yield
50	160	-1	-1	65.3
60	160	1	-1	68.2
50	170	-1	1	66.0
60	170	1	1	69.8
48	165	-1.414	0	64.5
62	165	1.414	0	69.0
55	158	0	-1.414	64.0
55	172	0	1.414	68.5
55	165	0	0	68.9
55	165	0	0	69.7
55	165	0	0	68.5
55	165	0	0	69.4
55	165	0	0	69.0

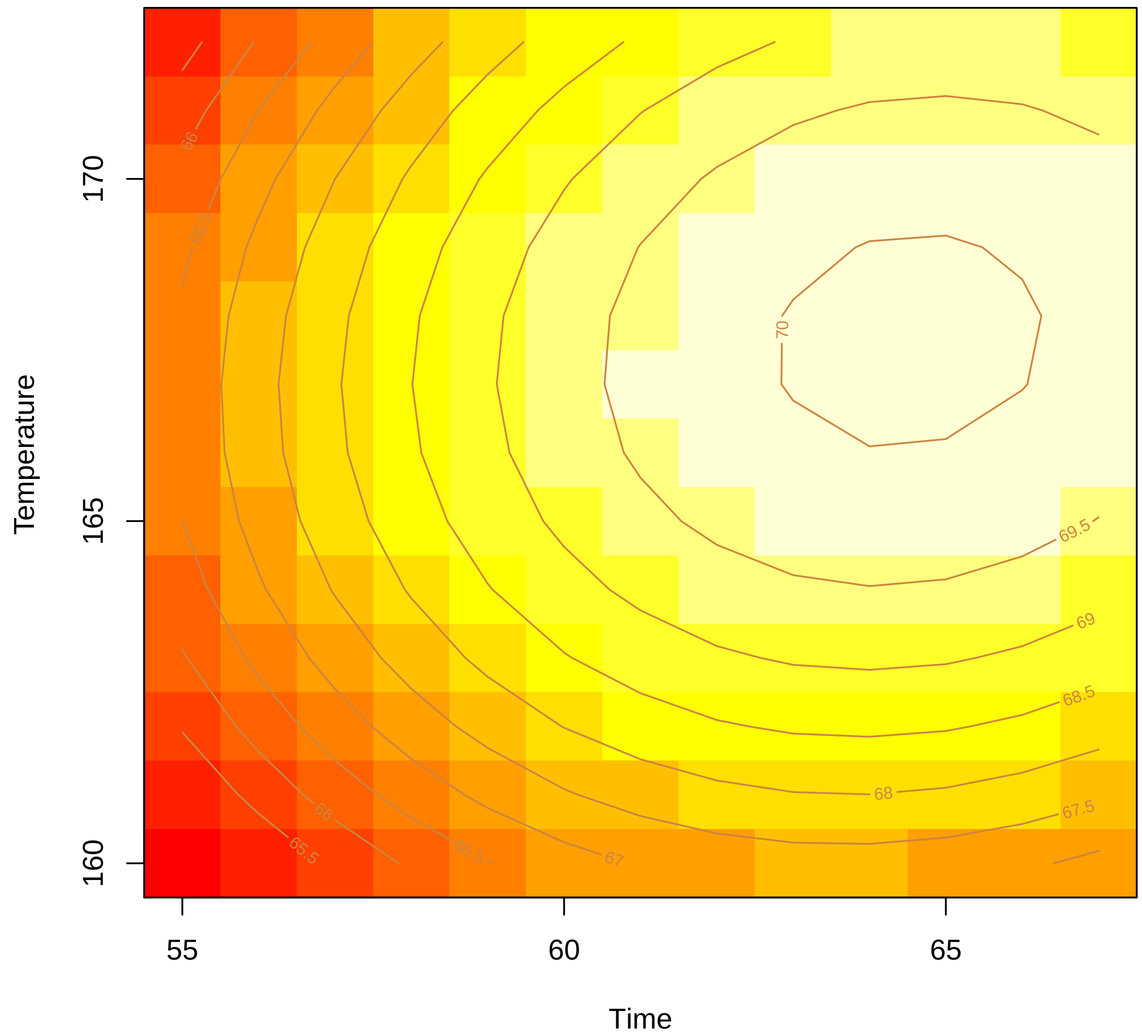
R Output

```
> summary(mod1)
Call: lm(formula=yield~x1+x2+I(x1^2)+I(x2^2)+x1*x2)
Coefficients:
               Value Std.Error  t value  Pr(>|t|)
(Intercept) 69.0999  0.3506   197.0815  0.0000
        x1   1.6331  0.2772     5.8913  0.0006
        x2   1.0830  0.2772     3.9070  0.0058
   I(x1^2)  -0.9688  0.2973    -3.2585  0.0139
   I(x2^2)  -1.2189  0.2973    -4.0996  0.0046
    x1:x2    0.2250  0.3920     0.5740  0.5839
Res. st.error: 0.784 on 7 df Mult R-Sq: 0.9143
F-statistic: 14.93 on 5 and 7 df, p-value 0.00129
```

Response surface



Contour lines



R code

```
mod1=lm(Yield~x1+x2+I(x1^2)+I(x2^2)+x1*x2,data=surf)
x=seq(-1,1.5,0.2); y=seq(-1,1.5,0.2)
f = function(x,y) {new.x=data.frame(x1=x,x2=y)
                   predict(mod1,new.x)}
z = outer(x,y,f)

persp(x,y,z,theta=30,phi=30,expand=0.5,col="lightblue",
xlab="Time",ylab="Temperature",zlab="Yield")

image(x,y,z,axes=F,xlab="Time",ylab="Temperature")
contour(x,y,z,levels=seq(65.5,80,by=0.5),add=T,col="peru")
axis(1,at=seq(-1,1,by=1),labels=c(55,60,65))
axis(2,at=seq(-1,1,by=1),labels=c(160,165,170))
box()
```