01NAEX - Lecture 09 3^k Factorial and Response Surface Design

Jiri Franc

Czech Technical University
Faculty of Nuclear Sciences and Physical Engineering
Department of Mathematics

3^k factorial design:

it is a factorial arrangement with k factors each at three levels, which are denoted by:

- low,
- 1 intermediate,
- 2 high.

Example:

consider the 3^2 design, quantitative factors, and let x_1 represent the factor A and x_2 represent factor B. A regression model relating the response y to x_1 and x_2 that is supported by this design is

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{122} x_1 x_2^2 + \beta_{112} x_1^2 x_2 + \beta_{1122} x_1^2 x_2^2 + \epsilon$$

Notice:

The addition of third factor level allows the relationship between the response and the design factors to be modeled as a quadratic. The two factor interaction *AB* is then subdividing into four single degree of freedom components.

We can label the design points, similar to what we did in 2^k factorial design.

However, the coding using $\{0,1,2\}$, which is a generalization of the $\{0,1\}$ coding that we also used in the 2^k design is more preferred.

Α	В	Α	В
-	-	0	0
0	-	1	0
+	-	2	0
-	0	0	1
0	0	1	1
+	0	2	1
-	+	0	2
0	+	1	2
+	+	2	2

 3^k factorial design allows to model a curvature in the response function. However, two points need to be considered.

- The 3^k design is not the most efficient way to model a quadratic relationship (the response surface designs are superior alternatives).
- 2. The 2^k design augmented with center points is an excellent way to obtain an indication of curvature. It allows one to keep the size and complexity of the design low and simultaneously obtain some protection against curvature. Then, if curvature is important, the 2^k design can be augmented with axial runs to obtain a central composite design.

Let us consider 3^2 factorial design. There are 8 DF between treatment combinations, where the main effects of A and B each have 2 DF, and the AB interaction has 4 DF.

If the factor is quantitative:

Each main effect can be represented by a linear and a quadratic component, each with a single degree of freedom. The two-factor interaction AB may be partitioned in two ways.

The first method consists of subdividing AB into the four single-degree-of-freedom components corresponding to $AB_{L\times L}$, $AB_{L\times Q}$, $AB_{Q\times L}$, and $AB_{Q\times Q}$. This can be done by fitting the terms β_{12} , β_{122} , β_{112} , and β_{1122} .

And for the interaction sum of squares hold:

$$SS_{AB} = SS_{AB_{LxL}} + SS_{AB_{LxQ}} + SS_{AB_{QxL}} + SS_{AB_{QxQ}}$$

where L denoted linear and Q quadratic.

The 3² Factorial Design - partitioning of the AB interaction

Another way how to subdivide the interaction *AB* is to use Latin Squares. This method doesn't require that the factors be quantitative and it is usually associated with the case where all factors are qualitative.

Since interactions in three level designs don't have the same number of degrees of freedom as main effects we must partition the interactions into pseudo components (pseudo factors) called the AB component and the AB^2 component. These components could be called pseudo-interaction effects.

The components are defined as a linear combination as follows:

Levels_{AB2} =
$$x_1 + x_2 (mod3)$$

Levels_{AB2} = $x_1 + 2x_2 (mod3)$

Pseudo components of decomposition of AB interaction in 3² design:

Levels_{AB} =
$$x_1 + x_2 \pmod{3}$$

Levels_{AB²} = $x_1 + 2x_2 \pmod{3}$

Α	В	AB	AB ²
0	0	0	0
1	0	1	1
2	0	2	2
0	1	1	2
1	1	2	0
2	1	0	1
0	2	2	1
1	2	0	2
2	2	1	0

The components AB and AB² each have two degrees of freedom. Note that

$$A^2B = (A^2B)^2 = A^4B^2 = AB^2$$
.

The partitioning has no actual meaning and is not displayed in ANOVA results, but is useful in constructing more complex designs.

The 3² Factorial Design - Latin Squares construction

Let us consider 3² factorial design. In latin square notation we obtain:

Latin block a =
$$AB$$
 component $Q: = x_1 + x_2 = 0 \pmod{3}$
 $R: = x_1 + x_2 = 1 \pmod{3}$
 $S: = x_1 + x_2 = 2 \pmod{3}$

Latin block b =
$$AB^2$$
 component $Q: = x_1 + 2x_2 = 0 \pmod{3}$
 $R: = x_1 + 2x_2 = 1 \pmod{3}$
 $S: = x_1 + 2x_2 = 2 \pmod{3}$
 $SS_{AB} = SS_A + SS_B$

The AB and AB^2 components have no physical significance and can be called as I and J components of interaction:

$$I(AB) = AB^2$$
$$J(AB) = AB$$

The effective life of a cutting tool installed in a numerically controlled machine is thought to be affected by the cutting speed and the tool angle.

Three speeds and three angles are selected, and a 3^2 factorial experiment with two replicates is performed.

Data for Tool Life Experiment							
Total Angle		Cutting Spec	ed (in/min)				
(degrees)	125	150	175	y _i			
15	$\begin{array}{ccc} -2 \\ -1 \end{array}$	$\begin{array}{ccc} -3 & & \\ 0 & & \end{array}$	² ₃ (5)	-1			
20	0 2	1 4	6 (10)	16			
25	$\begin{pmatrix} -1 \\ 0 \end{pmatrix}$	5 6 (1)	$\begin{pmatrix} 0 \\ -1 \end{pmatrix}$	9			
У.ј.	-2	12	14	24 = y			

Simple 3² Factorial Design - ANOVA with interaction.

summary(lm(Life~Angle*Speed, data=data_55))

Regression model with interaction.

Residual standard error: 2.483 on 14 degrees of freedom Multiple R-squared: 0.3038, Adjusted R-squared: 0.1546 F-statistic: 2.036 on 3 and 14 DF, p-value: 0.1551

Regression with quadratic terms and 4 interaction terms.

```
summary(lm(Life~Angle+Speed+Angle:Speed+I(Angle^2)+I(Speed^2)
   +I(Angle^2):Speed+I(Speed^2):Angle+I(Angle^2):I(Speed^2))
Coefficients:
                     Estim.Std. Error t value Pr(>|t|)
                    -1.068e+03 7.022e+02 -1.521 0.1626
(Intercept)
Angle
                     1.363e+02 7.261e+01 1.877 0.0932 .
Speed
                 1.448e+01 9.503e+00 1.524 0.1619
I(Angle^2) -4.080e+00 1.810e+00 -2.254 0.0507 .
          -4.960e-02 3.164e-02 -1.568 0.1514
I(Speed^2)
Angle:Speed
            -1.864e+00 9.827e-01 -1.897 0.0903 .
Speed:I(Angle^2) 5.600e-02 2.450e-02 2.285 0.0481 *
Angle:I(Speed^2) 6.400e-03 3.272e-03 1.956 0.0822 .
I(Angle^2):I(Speed^2) -1.920e-04 8.158e-05 -2.353 0.0431 *
Residual standard error: 1.202 on 9 degrees of freedom
Multiple R-squared: 0.8952, Adjusted R-squared: 0.802
F-statistic: 9.606 on 8 and 9 DF, p-value: 0.001337
```

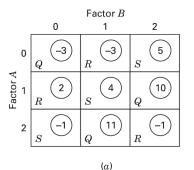
ANOVA with quadratic terms and 4 interaction terms.

```
summary(aov(lm(Life~Angle+Speed+Angle:Speed
+I(Angle^2)+I(Speed^2)+I(Angle^2):Speed+I(Speed^2):Angle
+I(Angle^2):I(Speed^2))))
```

	Df	Sum Sq	Mean Sq	F value Pr(>F)	
Angle	1	8.33	8.33	5.769 0.039772 *	
Speed	1	21.33	21.33	14.769 0.003948 **	
I(Angle^2)	1	16.00	16.00	11.077 0.008824 **	
I(Speed^2)	1	4.00	4.00	2.769 0.130451	
Angle:Speed	1	8.00	8.00	5.538 0.043065 *	
Speed:I(Angle^2)	1	2.67	2.67	1.846 0.207306	
Angle:I(Speed^2)	1	42.67	42.67	29.538 0.000414 ***	k
<pre>I(Angle^2):I(Speed^2)</pre>) 1	8.00	8.00	5.538 0.043065 *	
Residuals	9	13.00	1.44		

$$SS_{AB} = SS_{LXL} + SS_{LXQ} + SS_{QXL} + SS_{QXQ} = 8 + 42.67 + 2.67 + 8.00 = 61.34.$$

Interaction decomposition by Latin Squares



(b)

$$SS_{block \ a} = \frac{18^2 + (-2)^2 + 8^2}{(3)(2)} - \frac{24^2}{(9)(2)} = 33.34$$

 $SS_{block \ b} = \frac{0^2 + 6^2 + 18^2}{(3)(2)} - \frac{24^2}{(9)(2)} = 28.00$
 $SS_{AB} = SS_{block \ a} + SS_{block \ b} = 33.34 + 28.00 = 61.34$

In 3^3 design the two-factor interaction can be decomposed into eight single degree of freedom components (linear and quadratic combinations) or into four orthogonal two degree of freedom components, which are usually called W, X, Y, and Z.

$$\begin{array}{lcl} \textit{Levels}_{\textit{AB}^2\textit{C}^2} = \textit{W}(\textit{ABC}) : & = & \textit{x}_1 + 2\textit{x}_2 + 2\textit{x}_3 = 0 (\textit{mod}3) \\ \textit{Levels}_{\textit{AB}^2\textit{C}} = \textit{X}(\textit{ABC}) : & = & \textit{x}_1 + 2\textit{x}_2 + \ \textit{x}_3 = 0 (\textit{mod}3) \\ \textit{Levels}_{\textit{ABC}^2} = \textit{Y}(\textit{ABC}) : & = & \textit{x}_1 + \ \textit{x}_2 + 2\textit{x}_3 = 0 (\textit{mod}3) \\ \textit{Levels}_{\textit{ABC}} = \textit{Z}(\textit{ABC}) : & = & \textit{x}_1 + \ \textit{x}_2 + \ \textit{x}_3 = 0 (\textit{mod}3) \\ \end{array}$$

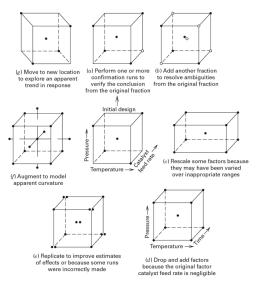
In general 3^k design, the only exponent allowed on the first letter is 1.

Like the I and J components, the W, X, Y, and Z components have no practical interpretation.

This decomposition is very useful, when we want to block 3^k design into 3^p blocks. We take one of the component of the interaction and confound it with blocks.

How to follow up experimentation

Iterative experimentation with alternatives for a subsequent set of runs depending on results from a previous set.



Response Surface Designs (RSD)

Response Surface Designs, sometime called Response Surface Methods (RSM), is a collection of techniques useful for modeling and analysis of problems in which a response of interest y is influenced by several variables x_1, x_2, \ldots, x_k and the goal is to optimize this response,

$$y = f(x_1, x_2, \ldots, x_k) + \varepsilon,$$

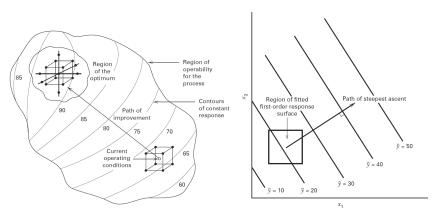
where ε represents the noise or error observed in the response y and

$$f(x_1,x_2,\ldots,x_k)=E[y]$$

is called a response surface.

Response Surface Designs (RSD)

RSD is a sequential procedure and frequently, the initial estimate of the optimum operating conditions is far from the actual optimum. The method of steepest ascent is a procedure for moving sequentially in the direction of the maximum increase in the response. We usually assume that in a small region of the x's is the response fitted by first-order model and the steepest ascent is a gradient procedure.



The yield *y* of a chemical process depends on reaction time *A* and temperature *B*. Current conditions are 35 min. and 155 F.

- Objective: Determine the operating conditions that maximize yield.
- ▶ Variables: Reaction Time & Temperature.
- ▶ Parameters: Time (30, 40) min, Temperature (150, 160) F.

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

$$x_2 = \frac{temperature - 155}{5}$$

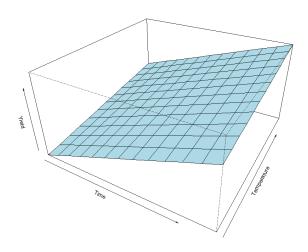
First order model:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon$$

```
> time = c(30, 40, 30, 40)
> temp = c(150, 150, 160, 160)
> vield = c(39.3, 40.9, 40.0, 41.5)
> x1 = (time - 35)/5
> x2 = (temp - 155)/5
> data11_1 = data.frame(time,temp,x1,x2,yield)
> summary(lm( yield \sim x1 + x2, data = data11 1))
Call:
lm.default(formula = yield \sim x1 + x2, data = data11 1)
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 degrees of freedom
Multiple R-squared: 0.9991, Adjusted R-squared: 0.9973
F-statistic: 565 on 2 and 1 DF, p-value: 0.02974
```

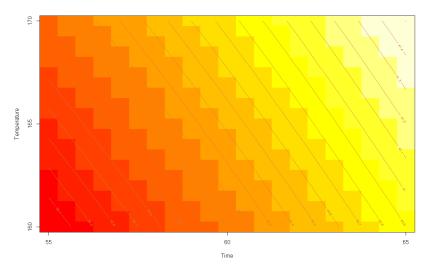
First order model:

$$y = 40.425 + 0.775x_1 + 0.325x_2$$



Contour plot of Yield process example for first order model:

$$y = 40.425 + 0.775x_1 + 0.325x_2$$



To estimate parameters in interaction model we have to add some center points, which

- ightharpoonup allows us to estimate the experimental error σ ,
- allows us to test the interaction effect,
- allows us to check for curvature.

Natural Variables		Co Vari	Response	
Ĕ 1	<i>ξ</i> ₂	x_1	x_2	y
30	150	-1	-1	39.3
30	160	-1	1	40.0
40	150	1	-1	40.9
40	160	1	1	41.5
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

We added four observations at the center to get an independent estimation of σ and check the fit of the first-order model or a curvature.

The replicates at the center can be used to calculate an estimate of experimental error σ^2 :

$$\hat{\sigma}^2 = MSE = \frac{\sum_{centerpoints} (y_i - \bar{y_c})^2}{n_c - 1} = \frac{0.172}{4} = 0.043$$

Second order model - checking for curvature

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

Estimation of curvature is an estimate for $\beta_{11}+\beta_{22}$

$$\bar{y}_F - \bar{y}_C = 40.425 - 40.46 = -0.035$$

Test of curvature

$$SS_{curv} = \frac{n_F n_C (\bar{y}_F - \bar{y}_C)^2}{n_F + n_C} = 0.0027$$

No evidence of Curvature (Pure quadratic effect), $F = \frac{SS_{curv}}{\hat{\sigma}_{2}^{2}} = 0.063$

Apply the method of steepest ascent on the first order model:

$$y = 40.425 + 0.775x_1 + 0.325x_2$$

Direction of steepest ascent - slope: $\frac{0.325}{0.775} = 0.42$

Step size in minutes: $\Delta x_1 = 5$

	Coded Variables		Natural	Response		
Steps	x_1	<i>x</i> ₂	<i>ξ</i> ₁	₹2	у	
Origin	0	0	35	155		
Δ	1.00	0.42	5	2		
Origin + Δ	1.00	0.42	40	157	41.0	
Origin + 2∆	2.00	0.84	45	159	42.9	
Origin + 3∆	3.00	1.26	50	161	47.1	
Origin + 4∆	4.00	1.68	55	163	49.7	
Origin + 5∆	5.00	2.10	60	165	53.8	
Origin + 6∆	6.00	2.52	65	167	59.9	
Origin + 7∆	7.00	2.94	70	169	65.0	
Origin + 8∆	8.00	3.36	75	171	70.4	
Origin + 9∆	9.00	3.78	80	173	77.6	
Origin + 10∆	10.00	4.20	85	175	80.3	
Origin + 11Δ	11.00	4.62	90	179	76.2	
Origin + 12∆	12.00	5.04	95	181	75.1	

Local minimum find in step 10 and we should run another first order model around this new conditions.

```
> x1 = (time - 85)/5
> x2 = (temp - 175)/5
> data11_3b = data.frame(time,temp,x1,x2,y1)
> data11 3b
  time temp x1 x2 y1
 80.00 170.00 -1.000 -1.000 76.5
  80.00 180.00 -1.000 1.000 77.0
  90.00 170.00 1.000 -1.000 78.0
  90.00 180.00 1.000 1.000 79.5
5 85.00 175.00 0.000 0.000 79.9
 85.00 175.00 0.000 0.000 80.3
7 85.00 175.00 0.000 0.000 80.0
8 85.00 175.00 0.000 0.000 79.7
 85.00 175.00 0.000 0.000 79.8
9
10 92.07 175.00 1.414 0.000 78.4
11 77.93 175.00 -1.414 0.000 75.6
12 85.00 182.07 0.000 1.414 78.5
13 85.00 167.93 0.000 -1.414 77.0
```

Linear regression model with interaction:

```
> summary(model3b)
Call:
lm.default(formula = y1 \sim x1 + x2 + I(x1^2) + I(x2^2) + x1:x2,
          data = data11 3b)
Residuals:
Min 1Q Median 3Q Max
-0.23995 -0.18089 -0.03995 0.17758 0.36005
Coefficients:
Estimate Std. Error t value Pr(>|t|)
x1 0.99505 0.09415 10.568 1.48e-05 ***
x2 0.51520 0.09415 5.472 0.000934 ***
I(x1^2) -1.37645 0.10098 -13.630 2.69e-06 ***
I(x2^2) -1.00134 0.10098 -9.916 2.26e-05 ***
x1:x2 0.25000 0.13315 1.878 0.102519
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 '' 1
Residual standard error: 0.2663 on 7 degrees of freedom
Multiple R-squared: 0.9827, Adjusted R-squared: 0.9704
F-statistic: 79.67 on 5 and 7 DF, p-value: 5.147e-06
```

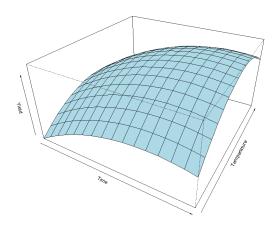
ANOVA of Linear regression model with interaction:

Linear regression model without interaction:

```
> summary (model3bb)
Call:
lm.default(formula = y1 \sim x1 + x2 + I(x1^2) + I(x2^2), data = data11_3
Residuals:
Min 1Q Median 3Q Max
-0.23995 -0.18089 -0.08232 0.06005 0.44808
Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept) 79.9400 0.1366 585.215 < 2e-16 ***
x1 0.9951 0.1080 9.213 1.56e-05 ***
x2 0.5152 0.1080 4.770 0.00141 **
I(x1^2) -1.3764 0.1158 -11.883 2.31e-06 ***
I(x2^2) -1.0013 0.1158 -8.645 2.49e-05 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
Residual standard error: 0.3054 on 8 degrees of freedom
Multiple R-squared: 0.974, Adjusted R-squared: 0.961
F-statistic: 75.02 on 4 and 8 DF, p-value: 2.226e-06
```

Model without interaction has some disadvantages. We can not use standard second order model and determine stationary points easily.

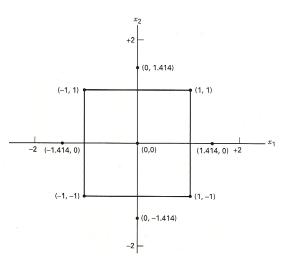
Location of stationary point - **Response surface plot** of Yield process example



The Second-Order Response Surface Model

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

Central composite design (CCD): optimization and fitting the model is easy.



The Second-Order Response Surface Model

$$\hat{\mathbf{y}} = \hat{\beta}_0 + \mathbf{x}^T \mathbf{b} + \mathbf{x}^T \mathbf{B} \mathbf{x},$$

where $\mathbf{x}^T = (x_1, x_2, \dots, x_k), \ \mathbf{b}^T = (\hat{\beta}_1, \dots, \hat{\beta}_k)$ and

$$\mathbf{B} = \begin{pmatrix} \hat{\beta}_{11} & \frac{\hat{\beta}_{12}}{2} & \cdots & \frac{\hat{\beta}_{1k}}{2} \\ \frac{\hat{\beta}_{12}}{2} & \hat{\beta}_{22} & \cdots & \frac{\hat{\beta}_{2k}}{2k} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\hat{\beta}_{1k}}{2} & \frac{\hat{\beta}_{1k}}{2} & \cdots & \hat{\beta}_{kk} \end{pmatrix}$$

The general mathematical solution for the location of the stationary point for fitted second order model is:

$$\frac{\partial \hat{y}}{\partial \mathbf{x}} = \mathbf{b} + 2\mathbf{B}\mathbf{x} = 0$$

$$\mathbf{x}_{\textit{stationary}} = -\frac{1}{2}\mathbf{B}^{-1}\mathbf{b}$$

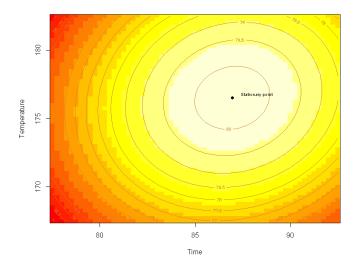
and the predicted response at the stationary point is:

$$\hat{y}_{stationary} = \hat{\beta}_0 + \frac{1}{2} \mathbf{x}_{stationary}^T \mathbf{b}$$

The Second-Order Response Surface Model

```
> b = matrix(c(model3b$coeff[2],model3b$coeff[3]),2,1)
> B = matrix(c(model3b$coeff[4], model3b$coeff[6]/2,
              model3b$coeff[6]/2,model3b$coeff[5]),2,2)
+
> cbind(b,B)
[,1] [,2] [,3]
[1,] 0.9950503 -1.376449 0.125000
[2,] 0.5152028 0.125000 -1.001336
> x_stat = -1/2 * solve(B) %*% b
> x_stat_natur = c((5*x_stat[1]+85), (5*x_stat[2]+175))
> y_stat_natur = predict (model3b,
                      data.frame(x1=x stat[1],x2=x stat[2]))
> x stat
[,1]
[1,] 0.3892304
[2,] 0.3058466
> x stat natur
[11] 86.94615 176.52923
> y_stat_natur
80.21239
```

Location of stationary point - Contour plot of Yield process example



Multiple Responses

Designs with multiple responses are common in practice. Typically, we want to simultaneously optimize all responses, or find a set of conditions where certain product properties are achieved.

A simple approach is to model all responses and overlay the contour plots.

Today Exercises

If necessary, continue in measurement to finish HW 02 from the last lesson.

, ,	x_1	x_2	x_3	y
	-1	-1	-1	66
	-1	-1	1	70
	-1	1	-1	78
Solve problems 11.8 from D.	-1	1	1	60
C. Montogomery DAOE.	1	-1	-1	80
T I 1.	1	-1	1	70
The data were collected in an	1	1	-1	100
experiment to optimize crystal	1	1	1	75
growth as a function of three	-1.682	0	0	100
variables x_1 , x_2 , and x_3 . Large	1.682	0	0	80
values of y (yield in grams) are	0	-1.682	0	68
desirable. Fit a second-order	0	1.682	0	63
model and analyze the fitted	0	0	-1.682	65
surface. Under what set of	0	0	1.682	82
conditions is maximum growth	0	0	0	113
achieved?	0	0	0	100
	0	0	0	118
	0	0	0	88
	0	0	0	100
	0	0	0	85

Today Exercises

	Run	Time (min)	Temperature (°C)	Catalyst (%)	Conversion (%) y ₁	Activity y ₂
	1	-1.000	-1.000	-1.000	74.00	53.20
	2	1.000	-1.000	-1.000	51.00	62.90
	3	-1.000	1.000	-1.000	88.00	53.40
Solve problems 11.12 from D.	4	1.000	1.000	-1.000	70.00	62.60
C. Montogomery DAOE.	5	-1.000	-1.000	1.000	71.00	57.30
o. Montogomery 27 to 2.	6	1.000	-1.000	1.000	90.00	67.90
Consider the three-variable	7	-1.000	1.000	1.000	66.00	59.80
	8	1.000	1.000	1.000	97.00	67.80
central composite design.	9	0.000	0.000	0.000	81.00	59.20
Analyze the data and draw	10	0.000	0.000	0.000	75.00	60.40
conclusions, assuming that we	11	0.000	0.000	0.000	76.00	59.10
wish to maximize conversion	12	0.000	0.000	0.000	83.00	60.60
(y_1) with activity (y_2) between	13	-1.682	0.000	0.000	76.00	59.10
	14	1.682	0.000	0.000	79.00	65.90
55 and 60 achieved?	15	0.000	-1.682	0.000	85.00	60.00
	16	0.000	1.682	0.000	97.00	60.70
	17	0.000	0.000	-1.682	55.00	57.40
	18	0.000	0.000	1.682	81.00	63.20
	19	0.000	0.000	0.000	80.00	60.80
	20	0.000	0.000	0.000	91.00	58.90