Section 1

MANE 6313

Subsection 1

Week 13, Module E

Student Learning Outcome

- Select an appropriate experimental design with one or more factors,
- Select an appropriate model with one or more factors,
- Evaluate statistical analyses of experimental designs,
- Assess the model adequacy of any experimental design, and
- Interpret model results.

Module Learning Outcome

Generate Box-Behnken Design in R

bbd() Function

rsm (version 2.10.3)

bbd: Generate a Box-Behnken design

Description

This function can generate a Box-Behnken design in 3 to 7 factors, and optionally will block it orthogonally if there are 4 or 5 factors. It can also randomize the design.

Usage

```
bbd(k, n0 = 4, block = (k == 4 | k == 5), randomize = TRUE, coding)
```

Arguments

k	A formula, or an integer giving the number of variables. If the formula has a left-hand side, the variables named there are appended to the design and initialized to `NA`.
n0	Number of center points in each block.
block	Logical value specifying whether or not to block the design; or a character string (taken as `TRUE`) giving the desired name for the blocking factor. Only BBDs with 4 or 5 factors can be blocked. A 4-factor BBD has three orthogonal blocks, and a 5-factor BBD has two.
randomize	Logical value determining whether or not to randomize the design. If `block` is `TRUE`, each block is randomized separately.
coding	Optional list of formulas. If this is provided, it overrides the default coding formulas.

Example Problem

- Taken from Dean, Voss, and Drajuljic (2016)[a]

11. Resin moisture experiment

A Box–Behnken design was used to determine whether specific drying conditions for a process could yield a resin that is sufficiently devoid of moisture and low-molecular-weight components. The three factors T, H, and P under study were temperature (150, 185, 220°C), relative humidity (0, 50, 100%), and air pressure (1, 5, 9 torr). The response variable y was a measure of product degradation (ppm). The design and data are shown in Table 16.27.

(a) Fit the second-order model, using coded factor levels.
(b) Test for model lack of fit.
(c) Check the equal-variance and normality model assumptions using residual plots.
(d) Conduct the canonical analysis.
(e) Conduct the analysis of variance.
(f) Summarize the results.

Figure 2: DVD Problem 16.11

[a] Dean, Voss, and Drajuljic (2017). Design and Analysis of Experiments, 2nd edition. Springer Texts in Statistics.

Example Problem, Data Table

Table 16.27 Resin degradation (ppm) for the resin moisture experiment

Design point	T		H		P		
	z_T	x_T	z_H	x_H	z_P	x_P	y
1	−1	150	−1	0	0	4	83
2	−1	150	0	50	−1	1	103
3	−1	150	0	50	1	9	94
4	−1	150	1	100	0	4	98
5	0	185	−1	0	−1	1	51
6	0	185	−1	0	1	9	48
7	0	185	1	100	−1	1	106
8	0	185	1	100	1	9	108
9	1	220	−1	0	0	4	36
10	1	220	0	50	−1	1	153
11	1	220	0	50	1	9	107
12	1	220	1	100	0	4	87
13	0	185	0	50	0	4	80
14	0	185	0	50	0	4	81
15	0	185	0	50	0	4	77
16	0	185	0	50	0	4	80
17	0	185	0	50	0	4	82

Figure 3: DVD Table 16.27

Coding Formula

$$x_1 \sim (temp - 185)/35$$
$$x_2 \sim (humidity - 50)/50$$
$$x_3 \sim (pressure - 5)/4$$

R Chunk for Box-Behnken Design

```
library(rsm)
bbd11.df <- bbd(3,n0=5,coding=list(x1~(temp-185)/35,x2~(humidi
y <- c(83,36,98,87,103,153,94,107,51,106,48,108,80,81,77,80,82
bbd11.df$y <- y
print(bbd11.df)
```

R Chunk for Box-Behnken Design Output

```r
library(rsm)
bbd11.df <- bbd(3,n0=5,coding=list(x1~(temp-185)/35,x2~(humidity-50)/50,x3~(pressure-5)/4),randomize = FALSE)
y <- c(83,36,98,87,103,153,94,107,51,106,48,108,80,81,77,80,82)
bbd11.df$y <- y
print(bbd11.df)
```

```
   run.order std.order temp humidity pressure   y
1          1         1  150        0        5  83
2          2         2  220        0        5  36
3          3         3  150      100        5  98
4          4         4  220      100        5  87
5          5         5  150       50        1 103
6          6         6  220       50        1 153
7          7         7  150       50        9  94
8          8         8  220       50        9 107
9          9         9  185        0        1  51
10        10        10  185      100        1 106
11        11        11  185        0        9  48
12        12        12  185      100        9 108
13        13        13  185       50        5  80
14        14        14  185       50        5  81
15        15        15  185       50        5  77
16        16        16  185       50        5  80
17        17        17  185       50        5  82

Data are stored in coded form using these coding formulas ...
x1 ~ (temp - 185)/35
x2 ~ (humidity - 50)/50
x3 ~ (pressure - 5)/4
```

R Chunk for Fitting Model

```
bbd11.model1 <- rsm(y~SO(x1,x2,x3),data=bbd11.df)
summary(bbd11.model1)
```

Model Output, part 1

```
Call:
rsm(formula = y ~ SO(x1, x2, x3), data = bbd11.df)

            Estimate Std. Error t value  Pr(>|t|)
(Intercept)  80.0000     8.4663  9.4492 3.104e-05 ***
x1            0.6250     6.6932  0.0934   0.92822
x2           22.6250     6.6932  3.3803   0.01175 *
x3           -7.0000     6.6932 -1.0458   0.33040
x1:x2         9.0000     9.4656  0.9508   0.37337
x1:x3        -9.2500     9.4656 -0.9772   0.36102
x2:x3         1.2500     9.4656  0.1321   0.89866
x1^2         16.0000     9.2260  1.7342   0.12647
x2^2        -20.0000     9.2260 -2.1678   0.06683 .
x3^2         18.2500     9.2260  1.9781   0.08843 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Multiple R-squared:  0.7851,    Adjusted R-squared:  0.5089
F-statistic: 2.842 on 9 and 7 DF,  p-value: 0.09117
```

Figure 5: Coefficients from bbd() Full Model

Model Output, part 2

```
Analysis of Variance Table

Response: y
                 Df Sum Sq Mean Sq  F value    Pr(>F)
FO(x1, x2, x3)    3 4490.3 1496.75   4.1763   0.05447
TWI(x1, x2, x3)   3  672.5  224.17   0.6255   0.62099
PQ(x1, x2, x3)    3 4004.0 1334.68   3.7241   0.06904
Residuals         7 2508.7  358.39
Lack of fit       3 2494.7  831.58 237.5952 5.828e-05
Pure error        4   14.0    3.50
```

Figure 6: ANOVA from bbd() Full Model

Model Output, part 3

```
Stationary point of response surface:
        x1         x2         x3
-0.1310656  0.5405119  0.1400549

Stationary point in original units:
     temp  humidity  pressure
180.41270  77.02560   5.56022

Eigenanalysis:
eigen() decomposition
$values
[1]  22.01452  12.82616 -20.59067

$vectors
           [,1]      [,2]        [,3]
x1  0.63484406 0.7623210  0.12585595
x2  0.05653266 0.1166241 -0.99156587
x3 -0.77056932 0.6366047  0.03094211
```

Model Refinement

- For this example, we will use $\alpha = 0.1$.
- Start with pure quadratic and work back to first order
  - For pure quadratic, x2 and x3 are statistically significant using $\alpha = 0.1$
  - For two-factor interactions, no factors are statistically significant
  - For first order, x2 is statistically significant
- Using hierarchy, the model will be FO(x2,x3)+PQ(x2,x3)

Second Model, R Chunk

```
bbd11.model2 <- rsm(y~FO(x2,x3)+PQ(x2,x3),data=bbd11.df)
summary(bbd11.model2)
```

Second Model, Output

```
Call:
rsm(formula = y ~ FO(x2, x3) + PQ(x2, x3), data = bbd11.df)

             Estimate Std. Error t value Pr(>|t|)
(Intercept)  86.7368     7.4888 11.5822 7.17e-08 ***
x2           22.6250     6.6632  3.3955 0.005314 **
x3           -7.0000     6.6632 -1.0505 0.314166
x2^2        -19.1579     9.1719 -2.0888 0.058704 .
x3^2         19.0921     9.1719  2.0816 0.059456 .
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Multiple R-squared:  0.6349,    Adjusted R-squared:  0.5133
F-statistic: 5.218 on 4 and 12 DF,  p-value: 0.01138

Analysis of Variance Table

Response: y
             Df Sum Sq Mean Sq F value  Pr(>F)
FO(x2, x3)    2 4487.1 2243.56  6.3165 0.01337
PQ(x2, x3)    2 2926.1 1463.07  4.1191 0.04346
Residuals    12 4262.3  355.19
Lack of fit   4 1748.8  437.19  1.3915 0.31941
```

Partial F- Test

```
51 ```{r}
52 anova(bbd11.model2,bbd11.model1)
53 ```
```

```
Analysis of Variance Table

Model 1: y ~ FO(x2, x3) + PQ(x2, x3)
Model 2: y ~ FO(x1, x2, x3) + TWI(x1, x2, x3) + PQ(x1, x2, x3)
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     12 4262.3
2      7 2508.7  5    1753.5 0.9785 0.4913
```

Figure 9: Partial F-test in R