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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

(1,5,9)

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

mistake

Design point	T		H		P		
	coded z_T	uncoded x_T	z_H	x_H	z_P	x_P	y
1	−1	150	−1	0	0	~~4~~ 5	83
2	−1	150	0	50	−1	1	103
3	−1	150	0	50	1	9	94
4	−1	150	1	100	0	~~4~~ 5	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

C.P.

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

center pts

```
library(rsm)
bbd11.df <- bbd(3,n0=5,coding=list(x1~(temp-185)/35,x2~(humid
y <- c(83,36,98,87,103,153,94,107,51,106,48,108,80,81,77,80,8
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

$\alpha = .1$

```
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
```

green terms removed from model

$FO(x_2, x_3) + PQ(x_2, x_3)$

$\underbrace{x_2^2, x_3^2, x_2, x_3}_{k=4}$

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
```

Lack of fit is Statistically significant

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

Coefficient

- 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

$\alpha = .1$

```
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
```

Lack of fit is not Statistically Significant

Partial F- Test

reduced

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

full

```
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
```

Since the p-value is large, we fail to reject H_0 and accept that all the terms had $\beta_k = 0$

Figure 9: Partial F-test in R

Remaining Analysis:
Residuals