Section 1

MANE 6313

Subsection 1

Week 14, Module F

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

Apply Sequential Analysis for CCD

Sequential Analysis in rsm()

- Package rsm() provides capabilities of adding center points and/or star points to factorial analysis
- Consider example for Dean, Voss and Draguljic[a]

Table 16.24 Purified lecithin yield and phosphatidylcholine enrichment (PCE), given extraction time (z_1), solvent volume (z_2), ethanol concentration (z_3), and temperature (z_4); fractionation experiment

Run	z_1	z_2	z_3	z_4	Yield	PCE
1	1	1	1	1	27.6	43.8
2	−1	−1	1	1	16.6	27.2
3	1	−1	−1	1	15.4	23.6
4	−1	1	−1	1	17.4	26.2
5	1	−1	1	−1	17.0	27.8
6	−1	1	1	−1	19.0	30.2
7	1	1	−1	−1	17.4	25.2
8	−1	−1	−1	−1	12.6	18.8
9	1	−1	1	1	18.6	28.8
10	−1	1	1	1	22.4	36.8
11	1	1	−1	1	21.4	33.4
12	−1	−1	−1	1	14.0	21.0
13	1	1	1	−1	24.0	38.0
14	−1	−1	1	−1	15.6	23.6
15	1	−1	−1	−1	13.0	20.2
16	−1	1	−1	−1	14.4	22.6
17	0	0	0	0	22.6	
18	$\sqrt{2}$	0	0	0	23.4	
19	$-\sqrt{2}$	0	0	0	20.6	
20	0	$\sqrt{2}$	0	0	22.6	

Initial Design

- The initial design is a single replicate of a 2^4 factorial with no center points

```
81 ```{r}
82 library(rsm)
83 sosada.df <- cube(4,n0=0,reps=1,randomize=FALSE)
84 print(sosada.df)
85 ```
```

```
   run.order std.order x1.as.is x2.as.is x3.as.is x4.as.is
1          1         1       -1       -1       -1       -1
2          2         2        1       -1       -1       -1
3          3         3       -1        1       -1       -1
4          4         4        1        1       -1       -1
5          5         5       -1       -1        1       -1
6          6         6        1       -1        1       -1
7          7         7       -1        1        1       -1
8          8         8        1        1        1       -1
9          9         9       -1       -1       -1        1
10        10        10        1       -1       -1        1
11        11        11       -1        1       -1        1
12        12        12        1        1       -1        1
13        13        13       -1       -1        1        1
14        14        14        1       -1        1        1
15        15        15       -1        1        1        1
16        16        16        1        1        1        1

Data are stored in coded form using these coding formulas ...
```

Initial Design with Response

x4 ~ x4.as.is

Subsection 2

```r
library(rsm)
Yield <- c(12.6,13.0,14.4,17.4,15.6,17.0,19.0,24.0,14.0,15.4,17.4,21.4,16.6,18.6,22.4,27.4)
sosada.df$Yield <- Yield
print(sosada.df)
```

```
   run.order std.order x1.as.is x2.as.is x3.as.is x4.as.is Yield
1          1         1       -1       -1       -1       -1  12.6
2          2         2        1       -1       -1       -1  13.0
3          3         3       -1        1       -1       -1  14.4
4          4         4        1        1       -1       -1  17.4
5          5         5       -1       -1        1       -1  15.6
6          6         6        1       -1        1       -1  17.0
7          7         7       -1        1        1       -1  19.0
8          8         8        1        1        1       -1  24.0
9          9         9       -1       -1       -1        1  14.0
10        10        10        1       -1       -1        1  15.4
11        11        11       -1        1       -1        1  17.4
12        12        12        1        1       -1        1  21.4
13        13        13       -1       -1        1        1  16.6
14        14        14        1       -1        1        1  18.6
15        15        15       -1        1        1        1  22.4
16        16        16        1        1        1        1  27.4

Data are stored in coded form using these coding formulas ...
```

x4 ~ x4.as.is

First Model

- Only coefficient information is shown
- Model can not be further refined

```r
library(rsm)
sosada.model1 <- rsm(Yield~FO(x1,x2,x3,x4)+TWI(x1,x2,x3,x4),data=sosada.df)
summary(sosada.model1)
```

```
Call:
rsm(formula = Yield ~ FO(x1, x2, x3, x4) + TWI(x1, x2, x3, x4),
    data = sosada.df)

            Estimate Std. Error  t value  Pr(>|t|)
(Intercept) 17.88750    0.06638 269.4729 1.336e-11 ***
x1           1.38750    0.06638  20.9025 4.642e-06 ***
x2           2.53750    0.06638  38.2271 2.308e-07 ***
x3           2.18750    0.06638  32.9544 4.836e-07 ***
x4           1.26250    0.06638  19.0194 7.405e-06 ***
x1:x2        0.73750    0.06638  11.1103 0.0001030 ***
x1:x3        0.28750    0.06638   4.3312 0.0074912 **
x1:x4        0.16250    0.06638   2.4480 0.0580761 .
x2:x3        0.58750    0.06638   8.8506 0.0003061 ***
x2:x4        0.46250    0.06638   6.9675 0.0009366 ***
x3:x4       -0.08750    0.06638  -1.3182 0.2446004
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 ' ' 0.1 ' ' 1
```

x4 ~ x4.as.is

Star Points

- One centerpoint and the axial points are added
- Since $\alpha = \sqrt{(2)}$, the value must inputted manually

```r
library(rsm)
sosada.design2 <- djoin(sosada.df,star(sosada.df,n0=1,alpha=1.41421,randomize=FALSE))
print(sosada.design2)
```

	run.order	std.order	x1.as.is	x2.as.is	x3.as.is	x4.as.is	Yield	Block
1	1	1	-1.00000	-1.00000	-1.00000	-1.00000	12.6	1
2	2	2	1.00000	-1.00000	-1.00000	-1.00000	13.0	1
3	3	3	-1.00000	1.00000	-1.00000	-1.00000	14.4	1
4	4	4	1.00000	1.00000	-1.00000	-1.00000	17.4	1
5	5	5	-1.00000	-1.00000	1.00000	-1.00000	15.6	1
6	6	6	1.00000	-1.00000	1.00000	-1.00000	17.0	1
7	7	7	-1.00000	1.00000	1.00000	-1.00000	19.0	1
8	8	8	1.00000	1.00000	1.00000	-1.00000	24.0	1
9	9	9	-1.00000	-1.00000	-1.00000	1.00000	14.0	1
10	10	10	1.00000	-1.00000	-1.00000	1.00000	15.4	1
11	11	11	-1.00000	1.00000	-1.00000	1.00000	17.4	1
12	12	12	1.00000	1.00000	-1.00000	1.00000	21.4	1
13	13	13	-1.00000	-1.00000	1.00000	1.00000	16.6	1
14	14	14	1.00000	-1.00000	1.00000	1.00000	18.6	1
15	15	15	-1.00000	1.00000	1.00000	1.00000	22.4	1
16	16	16	1.00000	1.00000	1.00000	1.00000	27.4	1
17	1	1	-1.41421	0.00000	0.00000	0.00000	NA	2
18	2	2	1.41421	0.00000	0.00000	0.00000	NA	2
19	3	3	0.00000	-1.41421	0.00000	0.00000	NA	2
20	4	4	0.00000	1.41421	0.00000	0.00000	NA	2
21	5	5	0.00000	0.00000	-1.41421	0.00000	NA	2

Augmented Design with Response

```{r}
augmentedYield <- c(12.6,13.0,14.4,17.4,15.6,17.0,19.0,24.0,14.0,15.4,17.4,21.4,16.6,18.6,22.4,27.4,20.6,23.4,13.4,22.6,15.6,15.6,17.6,21.0,22.6)
sosada.design2$augmentedYield <- augmentedYield
print(sosada.design2)
```

```
   run.order std.order x1.as.is x2.as.is x3.as.is x4.as.is Yield Block augmentedYield
1          1         1 -1.00000 -1.00000 -1.00000 -1.00000  12.6     1            12.6
2          2         2  1.00000 -1.00000 -1.00000 -1.00000  13.0     1            13.0
3          3         3 -1.00000  1.00000 -1.00000 -1.00000  14.4     1            14.4
4          4         4  1.00000  1.00000 -1.00000 -1.00000  17.4     1            17.4
5          5         5 -1.00000 -1.00000  1.00000 -1.00000  15.6     1            15.6
6          6         6  1.00000 -1.00000  1.00000 -1.00000  17.0     1            17.0
7          7         7 -1.00000  1.00000  1.00000 -1.00000  19.0     1            19.0
8          8         8  1.00000  1.00000  1.00000 -1.00000  24.0     1            24.0
9          9         9 -1.00000 -1.00000 -1.00000  1.00000  14.0     1            14.0
10        10        10  1.00000 -1.00000 -1.00000  1.00000  15.4     1            15.4
11        11        11 -1.00000  1.00000 -1.00000  1.00000  17.4     1            17.4
12        12        12  1.00000  1.00000 -1.00000  1.00000  21.4     1            21.4
13        13        13 -1.00000 -1.00000  1.00000  1.00000  16.6     1            16.6
14        14        14  1.00000 -1.00000  1.00000  1.00000  18.6     1            18.6
15        15        15 -1.00000  1.00000  1.00000  1.00000  22.4     1            22.4
16        16        16  1.00000  1.00000  1.00000  1.00000  27.4     1            27.4
17         1         1 -1.41421  0.00000  0.00000  0.00000    NA     2            20.6
18         2         2  1.41421  0.00000  0.00000  0.00000    NA     2            23.4
19         3         3  0.00000 -1.41421  0.00000  0.00000    NA     2            13.4
20         4         4  0.00000  1.41421  0.00000  0.00000    NA     2            22.6
21         5         5  0.00000  0.00000 -1.41421  0.00000    NA     2            15.6
22         6         6  0.00000  0.00000  1.41421  0.00000    NA     2            15.6
23         7         7  0.00000  0.00000  0.00000 -1.41421    NA     2            17.6
24         8         8  0.00000  0.00000  0.00000  1.41421    NA     2            21.0
25         9         9  0.00000  0.00000  0.00000  0.00000    NA     2            22.6

Data are stored in coded form using these coding formulas ...
x1 ~ x1.as.is
x2 ~ x2.as.is
x3 ~ x3.as.is
x4 ~ x4.as.is
```

x4 ~ x4.as.is

Model 2

```{r}
library(rsm)
sosada.model2 <- rsm(sosada.design2$augmentedYield~Block+SO(x1,x2,x3,x4),data=sosada.design2)
summary(sosada.model2)
```

```
Call:
rsm(formula = sosada.design2$augmentedYield ~ Block + SO(x1,
    x2, x3, x4), data = sosada.design2)

            Estimate Std. Error t value  Pr(>|t|)
(Intercept) 25.63754    3.00557  8.5300 1.321e-05 ***
Block2      -3.03754    1.75888 -1.7270  0.118245
x1           1.30799    0.31464  4.1572  0.002458 **
x2           2.68054    0.31464  8.5195 1.334e-05 ***
x3           1.75000    0.31464  5.5620  0.000351 ***
x4           1.25042    0.31464  3.9742  0.003234 **
x1:x2        0.73750    0.35177  2.0965  0.065487 .
x1:x3        0.28750    0.35177  0.8173  0.434865
x1:x4        0.16250    0.35177  0.4619  0.655084
x2:x3        0.58750    0.35177  1.6701  0.129236
x2:x4        0.46250    0.35177  1.3148  0.221102
x3:x4       -0.08750    0.35177 -0.2487  0.809145
x1^2        -0.30000    0.86167 -0.3482  0.735723
x2^2        -2.30001    0.86167 -2.6693  0.025654 *
x3^2        -3.50002    0.86167 -4.0619  0.002834 **
x4^2        -1.65001    0.86167 -1.9149  0.087771 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Multiple R-squared:  0.9522,    Adjusted R-squared:  0.8726
```

x4 ~ x4.as.is

Model 3

- $\alpha = 0.05$ used to determine if a terms should be kept in the model

```r
library(rsm)
sosada.model3 <- rsm(sosada.design2$augmentedYield~FO(x1,x2,x3,x4)+PQ(x2,x3),data=sosada.design2)
summary(sosada.model3)
```

```
Near-stationary-ridge situation detected -- stationary point altered
 Change 'threshold' if this is not what you intend

Call:
rsm(formula = sosada.design2$augmentedYield ~ FO(x1, x2, x3,
    x4) + PQ(x2, x3), data = sosada.design2)

            Estimate Std. Error t value  Pr(>|t|)
(Intercept) 21.04000    0.75609 27.8273 3.019e-16 ***
x1           1.30799    0.37805  3.4599 0.0027949 **
x2           2.68054    0.37805  7.0905 1.307e-06 ***
x3           1.75000    0.37805  4.6291 0.0002085 ***
x4           1.25042    0.37805  3.3076 0.0039153 **
x2^2        -1.08500    0.59775 -1.8151 0.0862003 .
x3^2        -2.28500    0.59775 -3.8227 0.0012467 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Multiple R-squared:  0.8621,    Adjusted R-squared:  0.8161
F-statistic: 18.75 on 6 and 18 DF,  p-value: 7.614e-07
```

x4 ~ x4.as.is

Partial F-test

```r
```{r}
library(rsm)
anova(sosada.model3,sosada.model2)
```
```

```
Analysis of Variance Table

Model 1: sosada.design2$augmentedYield ~ FO(x1, x2, x3, x4) + PQ(x2, x3)
Model 2: sosada.design2$augmentedYield ~ Block + FO(x1, x2, x3, x4) +
    TWI(x1, x2, x3, x4) + PQ(x1, x2, x3, x4)
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     18 51.451
2      9 17.819  9    33.632 1.8874  0.179
```

x4 ~ x4.as.is

Model 3 Discussion

- Partial F-test indicates all terms removed for model 2 when model 3 was created **all** are statistically not significant
- Bad design because lack of fit test is not avialable (see below)
  - Adding one or more centerpoints would allow Lack of Fit test to be performed (at least 2 replicated values required)
- Remaining analysis should be performed:
  - Residual analysis
  - Graphical analysis
  - Stationary point analysis

```
Analysis of Variance Table

Response: sosada.design2$augmentedYield
                    Df  Sum Sq Mean Sq F value   Pr(>F)
FO(x1, x2, x3, x4)   4 270.443  67.611 23.6536 5.83e-07
PQ(x2, x3)           2  51.187  25.594  8.9539 0.001999
Residuals           18  51.451   2.858
Lack of fit         18  51.451   2.858     NaN      NaN
Pure error           0   0.000     NaN
```