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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	

24 → single
replicate

factorial

A

↓ 1 center point
+ 8 axial points

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 >
```

4 factors
no center points

	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

Subsection 2

```

87 ~ ```{r}
88 library(rsm)
89 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)
90 sosada.df$Yield <- Yield
91 print(sosada.df)
92 ~ ```

```

	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 ...

First Model

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

```

95 > {r}
96 library(rsm)
97 sosada.model1 <- rsm(Yield~F0(x1,x2,x3,x4)+TWI(x1,x2,x3,x4),data=sosada.df)
98 summary(sosada.model1)
99 >

```

Call:

```

rsm(formula = Yield ~ F0(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	

← x3:x4

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Star Points

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

```

102 ~ ```{r}
103 library(rsm)
104 sosada.design2 <- djoin(sosada.df, star(sosada.df, n0=1, alpha=1.41421, randomize=FALSE))
105 print(sosada.design2)
106 ~ ```

```

Handwritten notes: "base design" with an arrow pointing to `sosada.df`; "centerpoints" with an arrow pointing to `n0=1`.

	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

```

95 > ""{r}
96 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)
97 sosada.design2$augmentedYield <- augmentedYield
98 print(sosada.design2)
99 > ""

```

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	12.6	1	12.6
2	2	2	1.00000	-1.00000	-1.00000	13.0	1	13.0
3	3	3	-1.00000	1.00000	-1.00000	14.4	1	14.4
4	4	4	1.00000	1.00000	-1.00000	17.4	1	17.4
5	5	5	-1.00000	-1.00000	1.00000	15.6	1	15.6
6	6	6	1.00000	-1.00000	1.00000	17.0	1	17.0
7	7	7	-1.00000	1.00000	1.00000	19.0	1	19.0
8	8	8	1.00000	1.00000	1.00000	24.0	1	24.0
9	9	9	-1.00000	-1.00000	-1.00000	14.0	1	14.0
10	10	10	1.00000	-1.00000	-1.00000	15.4	1	15.4
11	11	11	-1.00000	1.00000	-1.00000	17.4	1	17.4
12	12	12	1.00000	1.00000	-1.00000	21.4	1	21.4
13	13	13	-1.00000	-1.00000	1.00000	16.6	1	16.6
14	14	14	1.00000	-1.00000	1.00000	18.6	1	18.6
15	15	15	-1.00000	1.00000	1.00000	22.4	1	22.4
16	16	16	1.00000	1.00000	1.00000	27.4	1	27.4
17	1	1	-1.41421	0.00000	0.00000	NA	2	20.6
18	2	2	1.41421	0.00000	0.00000	NA	2	23.4
19	3	3	0.00000	-1.41421	0.00000	NA	2	13.4
20	4	4	0.00000	1.41421	0.00000	NA	2	22.6
21	5	5	0.00000	0.00000	-1.41421	NA	2	15.6
22	6	6	0.00000	0.00000	1.41421	NA	2	15.6
23	7	7	0.00000	0.00000	0.00000	-1.41421	NA	17.6
24	8	8	0.00000	0.00000	0.00000	1.41421	NA	21.0
25	9	9	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

factorial
cp + stop points

Model 2

```

116 # ""{r}
117 library(rsm)
118 sosada.model2 <- rsm(sosada.design2$augmentedYield~Block+S0(x1,x2,x3,x4),data=sosada.design2)
119 summary(sosada.model2)
120 # ""

```

Call:

```

rsm(formula = sosada.design2$augmentedYield ~ Block + S0(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

Model 3

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

```

122 * ````{r}
123 library(rsm)
124 sosada.model3 <- rsm(sosada.design2$augmentedYield~F0(x1,x2,x3,x4)+PQ(x2,x3),data=sosada.design2)
125 summary(sosada.model3)
126 * ````

```

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

Call:

```
rsm(formula = sosada.design2$augmentedYield ~ F0(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

Reduced

warning

can not refine further

Partial F-test

```
129 ~ ```{r}
130 library(rsm)
131 anova(sosada.model3, sosada.model2)
132 ~ ```
```

Analysis of Variance Table

Model 1: sosada.design2\$augmentedYield ~ F0(x1, x2, x3, x4) + PQ(x2, x3)

Model 2: sosada.design2\$augmentedYield ~ Block + F0(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
---	---	--------	---	--------	--------	-------

remove all terms
in the list of
variables not
significant

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 available (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)
F0(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		