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Section 1

MANE 6313

Subsection 1

Week 14, Module A

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

Evaluate central composite designs using R

Central Composite Design in R

rsm (version 2.10.3)

ccd: Generate central-composite designs and associated building blocks

Description

These functions generate central-composite designs, or building blocks thereof. They allow for flexible choices of replications, aliasing of predictors and fractional blocks, and choices of axis or 'star' points.

Usage

```
cube(basis, generators, n0 = 4, reps = 1, coding, randomize = TRUE,
      blockgen, bid = 1, inscribed = FALSE)
star(basis, n0 = 4, alpha = "orthogonal", reps = 1, randomize = TRUE)
dupe(design, randomize = TRUE, coding)
foldover(basis, variables, bid, randomize = TRUE)
ccd(basis, generators, blocks = "Block", n0 = 4, alpha = "orthogonal",
     wbreps = 1, bbreps = 1, randomize = TRUE, inscribed = FALSE,
     coding, oneblock = FALSE)
```

ccd.pick()

ccd.pick: Find a good central-composite design

Description

This function looks at all combinations of specified design parameters for central-composite designs, calculates other quantities such as the '**alpha**' values for rotatability and orthogonal blocking, imposes specified restrictions, and outputs the best combinations in a specified order. This serves as an aid in identifying good designs. The design itself can then be generated using '**ccd**' or in pieces using '**cube**', '**star**', etc.

Usage

```
ccd.pick(k, n.c = 2^k, n0.c = 1:10, blks.c = 1, n0.s = 1:10, bbr.c = 1,
        wbr.s = 1, bbr.s = 1, best = 10, sortby = c("agreement", "N"),
        restrict)
```

Arguments

k	Number of factors in the design
n.c	Number(s) of factorial points in each cube block
n0.c	Numbers(s) of center points in each cube block
blks.c	Number(s) of cube blocks that together comprise one rep of the cube portion
n0.s	Numbers(s) of center points in each star (axis-point) block
bbr.c	Number(s) of copies of each cube block
wbr.s	Number(s) of replications of each star point within a block
bbr.s	Number(s) of copies of each star block
best	How many designs to list. Use ' best=NULL ' to list them all
sortby	String(s) containing numeric expressions that are each evaluated and used as sorting key(s). Specify ' sortby=NULL ' if no sorting is desired.

Example Problem

Table 4.7 Original and Coded Levels of Independent Variables

Variable	Original	Coded				
		-2	-1	0	1	2
Heating temperature	X_1 ($^{\circ}\text{C}/30$ min)	65.0	70.0	75.0	80.0	85.0
pH	X_2	4.0	5.0	6.0	7.0	8.0
Redox potential	X_3 (volt)	-0.025	0.075	0.175	0.275	0.375
Sodium oxalate	X_4 (Molar)	0.0	0.0125	0.025	0.0375	0.05
Sodium lauryl sulfate	X_5 (% of solids)	0.0	0.05	0.10	0.15	0.20

Source: S. H. Richert, C. V. Morr, and C. M. Cooney (1974). Reprinted from Journal of Food Science. Copyright © by Institute of Food Technologies.

Data from Example Problem

Table 4.6 Experimental Design (Coded) and Response Values

x_1	x_2	x_3	x_4	x_5	$Y(\%)$
-1	-1	-1	-1	1	80.6
1	-1	-1	-1	-1	67.9
-1	1	-1	-1	-1	83.1
1	1	-1	-1	1	38.1
-1	-1	1	-1	-1	79.7
1	-1	1	-1	1	74.7
-1	1	1	-1	1	71.2
1	1	1	-1	-1	36.8
-1	-1	-1	1	-1	81.7
1	-1	-1	1	1	66.8
-1	1	-1	1	1	73.0
1	1	-1	1	-1	40.5
-1	-1	1	1	1	74.9
1	-1	1	1	-1	74.2
-1	1	1	1	-1	63.5
1	1	1	1	1	42.8
-2	0	0	0	0	80.9
2	0	0	0	0	42.4
0	-2	0	0	0	73.4
0	2	0	0	0	45.0
0	0	-2	0	0	66.0
0	0	2	0	0	71.7
0	0	0	-2	0	77.5
0	0	0	2	0	76.3
0	0	0	0	-2	67.4
0	0	0	0	2	86.5
0	0	0	0	0	77.4
0	0	0	0	0	74.6
0	0	0	0	0	79.8
0	0	0	0	0	78.3
0	0	0	0	0	74.8

5 factors
 $2^5 - 1 \rightarrow 16 \text{ runs}$

fractional
 $1/16$

axial
 1056 points

$n_c = 5$

Source: S. H. Richert, C. V. Morr, and C. M. Cooney (1974). Reprinted from Journal of Food Science. Copyright © by Institute of

ccd() to Create Data Frame

```

98 > library(rsm)
99 ccd1.coded <- ccd(4, n0=c(0,6), alpha="rotatable", randomize=FALSE, generators=x5-x1*x2*x3*x4)
100 print(ccd1.coded)
101
102

```

run.order	std.order	x1.as.is	x2.as.is	x3.as.is	x4.as.is	x5.as.is	Block
1	1	1	-1	-1	-1	1	1
2	2	2	1	-1	-1	-1	1
3	3	3	-1	1	-1	-1	1
4	4	4	1	1	-1	-1	1
5	5	5	-1	-1	1	-1	1
6	6	6	1	-1	1	-1	1
7	7	7	-1	1	1	-1	1
8	8	8	1	1	1	-1	1
9	9	9	-1	-1	-1	1	1
10	10	10	1	-1	-1	1	1
11	11	11	-1	1	-1	1	1
12	12	12	1	1	-1	1	1
13	13	13	-1	-1	1	1	1
14	14	14	1	-1	1	1	1
15	15	15	-1	1	1	-1	1
16	16	16	1	1	1	1	1
17	1	1	-2	0	0	0	2
18	2	2	2	0	0	0	2
19	3	3	0	-2	0	0	2
20	4	4	0	2	0	0	2
21	5	5	0	0	-2	0	2
22	6	6	0	0	2	0	2
23	7	7	0	0	0	-2	2
24	8	8	0	0	0	2	2
25	9	9	0	0	0	0	-2
26	10	10	0	0	0	0	2
27	11	11	0	0	0	0	2
28	12	12	0	0	0	0	2
29	13	13	0	0	0	0	2
30	14	14	0	0	0	0	2
31	15	15	0	0	0	0	2
32	16	16	0	0	0	0	2

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

```

x1 ~ x1.as.is
x2 ~ x2.as.is
x3 ~ x3.as.is

```

$x_5 = x_1 x_2 x_3 x_4$

$n_0 \rightarrow$ center points
 $(0, 6)$
 0 in factorial
 6 on center points

Factorial

Star points
 + center points

Warm-up Design
 to understand
 concept,

but not
 useable

ccd() with Uncoded Data

```

104 > library(rsm)
105 ccd1.df <- ccd(~x1+x2+x3+x4,n0=c(0,6),alpha="rotatable",randomize=FALSE,coding =
106 list(x1=(Temp-75)/5,x2=(pH-6),x3=(redox-0.175)/0.1,x4=(naOxalate-0.025)/0.0125,x5=(naLauryl-0.1)/0.05),oneblock=TRUE,
107 E,generators=x5-x1*x2*x3*x4)
108 > print(ccd1.df)

```

run.order	std.order	Temp	pH	redox	naOxalate	naLauryl
1	1	1	70	5	0.075	0.0125
2	2	2	80	5	0.075	0.0125
3	3	3	70	7	0.075	0.0125
4	4	4	80	7	0.075	0.0125
5	5	5	70	5	0.275	0.0125
6	6	6	80	5	0.275	0.0125
7	7	7	70	7	0.275	0.0125
8	8	8	80	7	0.275	0.0125
9	9	9	70	5	0.075	0.0375
10	10	10	80	5	0.075	0.0375
11	11	11	70	7	0.075	0.0375
12	12	12	80	7	0.075	0.0375
13	13	13	70	5	0.275	0.0375
14	14	14	80	5	0.275	0.0375
15	15	15	70	7	0.275	0.0375
16	16	16	80	7	0.275	0.0375
17	1	1	65	6	0.175	0.0250
18	2	2	85	6	0.175	0.0250
19	3	3	75	4	0.175	0.0250
20	4	4	75	8	0.175	0.0250
21	5	5	75	6	-0.025	0.0250
22	6	6	75	6	0.375	0.0250
23	7	7	75	6	0.175	0.0000
24	8	8	75	6	0.175	0.0500
25	9	9	75	6	0.175	0.0250
26	10	10	75	6	0.175	0.0250
27	11	11	75	6	0.175	0.0250
28	12	12	75	6	0.175	0.0250
29	13	13	75	6	0.175	0.0250
30	14	14	75	6	0.175	0.0250
31	15	15	75	6	0.175	0.0250
32	16	16	75	6	0.175	0.0250

Right
Design

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

$x_1 \sim (\text{Temp} - 75)/5$

$x_2 \sim (\text{pH} - 6)$

$x_3 \sim (\text{redox} - 0.175)/0.1$

Adding Response Variable

```

110 ~ ```{r}
111 library(rsm)
112 Y <- c(80.6,67.9,83.1,38.1,79.7,74.7,71.2,36.8,81.7,66.8,73.0,40.5,74.9,74.2,63.5,42.8,80.9,42.4,73.4,45.0,66.0,71.
113       7,77.5,76.3,67.4,86.5,77.4,74.6,79.8,78.3,74.8,80.9)
114 ccd1.df$Y <- Y
115 ~```

```



run.order	std.order	Temp	pH	redox	naOxalate	naLauryl	Y
1	1	1	70	5	0.075	0.0125	0.15 80.6
2	2	2	80	5	0.075	0.0125	0.05 67.9
3	3	3	70	7	0.075	0.0125	0.05 83.1
4	4	4	80	7	0.075	0.0125	0.15 38.1
5	5	5	70	5	0.275	0.0125	0.05 79.7
6	6	6	80	5	0.275	0.0125	0.15 74.7
7	7	7	70	7	0.275	0.0125	0.15 71.2
8	8	8	80	7	0.275	0.0125	0.05 36.8
9	9	9	70	5	0.075	0.0375	0.05 81.7
10	10	10	80	5	0.075	0.0375	0.15 66.8
11	11	11	70	7	0.075	0.0375	0.15 73.0
12	12	12	80	7	0.075	0.0375	0.05 40.5
13	13	13	70	5	0.275	0.0375	0.15 74.9
14	14	14	80	5	0.275	0.0375	0.05 74.2
15	15	15	70	7	0.275	0.0375	0.05 63.5
16	16	16	80	7	0.275	0.0375	0.15 42.8
17	1	1	65	6	0.175	0.0250	0.10 80.9
18	2	2	85	6	0.175	0.0250	0.10 42.4
19	3	3	75	4	0.175	0.0250	0.10 73.4
20	4	4	75	8	0.175	0.0250	0.10 45.0
21	5	5	75	6	-0.025	0.0250	0.10 66.0
22	6	6	75	6	0.375	0.0250	0.10 71.7
23	7	7	75	6	0.175	0.0000	0.10 77.5
24	8	8	75	6	0.175	0.0500	0.10 76.3
25	9	9	75	6	0.175	0.0250	0.00 67.4
26	10	10	75	6	0.175	0.0250	0.20 86.5
27	11	11	75	6	0.175	0.0250	0.10 77.4
28	12	12	75	6	0.175	0.0250	0.10 74.6
29	13	13	75	6	0.175	0.0250	0.10 79.8
30	14	14	75	6	0.175	0.0250	0.10 78.3
31	15	15	75	6	0.175	0.0250	0.10 74.8
32	16	16	75	6	0.175	0.0250	0.10 80.9

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

x1 ~ (Temp - 75)/5

x2 ~ (pH - 6)

x3 ~ (redox - 0.175)/0.1

First Model - Coefficients

```

125 > library(rsm)
126 library(rsm)
127 ccd1.model1 <- rsm(Y~S0(x1,x2,x3,x4,x5),data=ccd1.df)
128 summary(ccd1.model1)
129 >

```

Call:
rsm(formula = Y ~ S0(x1, x2, x3, x4, x5), data = ccd1.df)

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	77.79432	1.85745	41.8823	1.750e-13 ***
x1	-10.12083	0.95058	-10.6470	3.938e-07 ***
x2	-8.67917	0.95058	-9.1304	1.821e-06 ***
x3	-0.10417	0.95058	-0.1096	0.9147145
x4	-0.71250	0.95058	-0.7495	0.4692583
x5	1.37083	0.95058	1.4421	0.1771350
x1:x2	-6.20625	1.16422	-5.3308	0.0002408 ***
x1:x3	2.76875	1.16422	2.3782	0.0366173 *
x1:x4	1.76875	1.16422	1.5193	0.1569046
x1:x5	0.70625	1.16422	0.6066	0.5564099
x2:x3	-1.68125	1.16422	-1.4441	0.1765837
x2:x4	-0.25625	1.16422	-0.2201	0.8298214
x2:x5	0.48125	1.16422	0.4134	0.6872818
x3:x4	0.04375	1.16422	0.0376	0.9706968
x3:x5	1.50625	1.16422	1.2938	0.2222458
x4:x5	0.03125	1.16422	0.0268	0.9790665
x1^2	-4.15682	0.85983	-4.8344	0.0005236 ***
x2^2	-4.76932	0.85983	-5.5468	0.0001736 ***
x3^2	-2.35682	0.85983	-2.7410	0.0191965 *
x4^2	-0.34432	0.85983	-0.4004	0.6964946
x5^2	-0.33182	0.85983	-0.3859	0.7069228

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

First Model - Anova

Analysis of Variance Table

Response: Y

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
FO(x1, x2, x3, x4, x5)	5	4323.8	864.75	39.8751	1.1e-06
TWI(x1, x2, x3, x4, x5)	10	883.3	88.33	4.0730	0.0149793
PQ(x1, x2, x3, x4, x5)	5	1179.8	235.97	10.8809	0.0005774
Residuals	11	238.6	21.69		
Lack of fit	6	205.5	34.24	5.1737	0.0458642
Pure error	5	33.1	6.62		

Stationary point of response surface:

x1	x2	x3	x4	x5
-0.394479	-0.624541	1.135045	-1.575681	3.694937

Stationary point in original units:

Temp	pH	redox	naOxalate	naLauryl
73.027604848	5.375458965	0.288504539	0.005303989	0.284746826

Eigenanalysis:

eigen() decomposition

\$values

[1] 0.5974405 -0.2085975 -1.0427378 -3.6500412 -7.6551549

\$vectors

	[,1]	[,2]	[,3]	[,4]	[,5]
x1	0.4752854	-0.10058397	0.3809698	0.3867462	0.68503720
x2	-0.3351535	0.09775804	-0.4170033	-0.4292114	0.72111121
x3	0.4385796	0.15056861	0.3971482	-0.7899316	-0.05708322
x4	0.5097058	-0.63801217	-0.5611295	-0.1156766	-0.06995046
x5	0.4578470	0.74202143	-0.4564836	0.1607000	-0.05070604

Concerning!
there is a statistically
significant LOF
in this model

Model Refinement

- Used $\alpha = 0.05$ for decision making
- **Terms to Keep** ~~(8)~~ **7**
 - $x_1, x_2, x_3, x_1:x_2, x_1:x_3, x_1^2, x_2^2, x_3^2$
- **Terms to Remove** ~~(12)~~ **13**
 - $x_4, x_5, x_1:x_4, x_1:x_5, x_2:x_3, x_2:x_4, x_2:x_5, x_3:x_4, x_3:x_5, x_4:x_5, x_4^2, x_5^2$

Reduced Model

```

135 ~ ```{r}
136 library(rsm)
137 ccd1.model2 <- rsm(Y~FO(x1,x2,x3)+TWI(x1,x2,x3)+PQ(x1,x2,x3),data=ccd1.df)
138 summary(ccd1.model2)
139 ~ ```

```

Call:

```
rsm(formula = Y ~ FO(x1, x2, x3) + TWI(x1, x2, x3) + PQ(x1, x2,
x3), data = ccd1.df)
```

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	77.17019	1.32414	58.2794	< 2.2e-16 ***
x1	-10.12083	0.87166	-11.6110	7.466e-11 ***
x2	-8.67917	0.87166	-9.9571	1.305e-09 ***
x3	-0.10417	0.87166	-0.1195	0.905961
x1:x2	-6.20625	1.06756	-5.8135	7.542e-06 ***
x1:x3	2.76875	1.06756	2.5935	0.016581 *
x2:x3	-1.68125	1.06756	-1.5749	0.129562
x1^2	-4.10481	0.78337	-5.2399	2.953e-05 ***
x2^2	-4.71731	0.78337	-6.0218	4.632e-06 ***
x3^2	-2.30481	0.78337	-2.9422	0.007538 **

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

Multiple R-squared: 0.9395, Adjusted R-squared: 0.9147
F-statistic: 37.93 on 9 and 22 DF, p-value: 2.369e-11

Analysis of Variance Table

Response: Y

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
FO(x1, x2, x3)	3	4266.5	1422.16	77.9912	7.018e-12
TWI(x1, x2, x3)	3	784.2	261.39	14.3345	2.144e-05
PQ(x1, x2, x3)	3	1173.6	391.22	21.4543	9.926e-07
Residuals	22	401.2	18.23		
Lack of fit	5	69.4	13.87	0.7107	0.6237

no lack of Fit

Partial F-test

```

142 > ```{r}
143 anova(ccd1.model2,ccd1.model1)
144 > ```

```

Analysis of Variance Table

Model 1: $Y \sim F0(x1, x2, x3) + TWI(x1, x2, x3) + PQ(x1, x2, x3)$

Model 2: $Y \sim F0(x1, x2, x3, x4, x5) + TWI(x1, x2, x3, x4, x5) + PQ(x1, x2, x3, x4, x5)$

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	22	401.17				
2	11	238.55	11	162.62	0.6817	0.7322

Fail to reject H_0 ,
and accept H_0 that
all ~~steps~~ for
variable in remove
list are not
statistically