Section 1

MANE 6313

Subsection 1

Week 14, Module D

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

Estimate stationary points from CCD model

Reduced Model from Module A

```r
library(rsm)
ccd1.model2 <- rsm(Y~FO(x1,x2,x3)+TWI(x1,x2,x3)+PQ(x1,x2,x3),data=ccd1.df)
summary(ccd1.model2)
```

```
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
```

Stationary Points from Reduced Model (Module A)

```
Stationary point of response surface:
       x1        x2        x3
-4.838989  2.978817 -4.015574

Stationary point in original units:
      Temp          pH      redox
50.8050558  8.9788169 -0.2265574

Eigenanalysis:
eigen() decomposition
$values
[1] -0.1255313 -3.4527009 -7.5486908

$vectors
          [,1]       [,2]       [,3]
x1  0.6136376 -0.3979581  0.6819665
x2 -0.5229922  0.4422168  0.7286449
```

First Derivatives

$$\hat{y} = 77.17 - 10.12x_1 - 8.68x_2 - .10x_3 - 6.21x_1x_2 + 2.77x_1x_3 - 1.68x_2x_3 - 4.10x_1^2 - 4.72x_2^2 - 2.30x_3^2$$

To find Stationary point solve $\frac{d\hat{y}}{dx} = 0$ (3 equations)

$$\frac{d\hat{y}}{dx_1} = -10.12 - 6.21x_2 + 2.77x_3 - 8.2x_1$$

$$\frac{d\hat{y}}{dx_2} = -8.68 - 6.21x_1 - 1.68x_3 - 9.44x_2$$

$$\frac{d\hat{y}}{dx_3} = ~~-6.2~~ - .1 + 2.77x_1 - 1.68x_2 - 4.6x_3$$

Matrix Formulation

Solve

$$Ax = b$$

where

$$A = \begin{bmatrix} -8.2 & -6.21 & 2.77 \\ -6.21 & -7.44 & -1.68 \\ 2.77 & -1.68 & -4.6 \end{bmatrix} \quad b = \begin{bmatrix} 10.12 \\ 8.68 \\ 0.1 \end{bmatrix}$$

Matrix Solution

```
183 ```{r}
184 b=matrix(c(10.12,8.68,0.104),3,1,byrow=TRUE)
185 A=matrix(c(-8.2,-6.21,2.77,-6.21,-9.44,-1.68,2.77,-1.68,-4.6),3,3,byrow=TRUE)
186 solution <- solve(A,b)
187 print(solution)
188 ```
```

```
           [,1]
[1,] -4.992283
[2,]  3.105502
[3,] -4.163015
```

- Compare to R software output

Uncoded Solution

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

Uncoded Solution

Stationary Point $x_1 = -4.838989$

$$\frac{\text{Temp} - 75}{5} = -4.838989$$

$$\text{Temp} = 75 - 4.838989(5)$$

$$= 50.805$$