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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

```

135 > {r}
136 library(rsm)
137 ccd1.model2 <- rsm(Y~F0(x1,x2,x3)+TWI(x1,x2,x3)+PQ(x1,x2,x3),data=ccd1.df)
138 summary(ccd1.model2)
139 >

```

Call:
 rsm(formula = Y ~ F0(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)
F0(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

$$\hat{y} = f(x_1, x_2, x_3)$$

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)

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

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

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

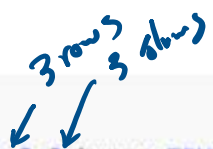
Matrix Formulation

Solve $Ax = b$ for $x \rightarrow A^{-1}Ax = A^{-1}b$
 $x = A^{-1}b$

where $A = \begin{bmatrix} -8.2 & -6.21 & 2.77 \\ -6.21 & -9.44 & -1.68 \\ 2.77 & -1.68 & -4.61 \end{bmatrix}$ $b = \begin{bmatrix} 10.12 \\ 8.68 \\ 0.1 \end{bmatrix}$

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 ...

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

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

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

$$x_4 \sim (\text{naOxalate} - 0.025)/0.0125$$

$$x_5 \sim (\text{naLauryl} - 0.1)/0.05$$

Uncoded Solution

Stationary Point $x_1 = -4.838989$
(computer output)

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

$$\begin{aligned}\text{Temp} &= 75 - 4.838989(5) \\ &= 50.805\end{aligned}$$