Lecture 15: Response Surface Methods

Montgomery: Chapter 11

Response Surface Methodology

- Response y and factors \mathbf{x}
- Factors influence response in unknown way
- Describe influence using model $f(\mathbf{x})$
- Objective is to find levels which maximize response

$$y = f(x_1, x_2, \dots, x_k) + \epsilon$$

- ϵ represents noise or error in response
- Call $\eta = f(x_1, x_2, \dots, x_k)$ the response surface
- Maximize response by maximizing response surface
- Contours values of $\mathbf x$ such that η is constant

1st and 2nd Order Approximations

- Use suitable approximation of f to maximize
 - First order Linear function of factors

$$y = \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k + \epsilon$$

- Second order - Quadratic function of factors

$$y = \beta_0 + \sum \beta_i x_i + \sum \beta_{ii} x_i^2 + \sum \sum \beta_{ij} x_i x_j + \epsilon$$

- While two approximations unrealistic in general
- Often quite realistic in small region of surface
- Use sequential approach to find optimum
 - 1. Response surface design determines $\{x_i\}$
 - 2. Least squares to estimate parameters
 - 3. Use contours to move in optimal direction

The Method of Steepest Ascent

- Move rapidly to general vicinity of optimum
- Use approximate model to move in proper direction
- Consider linear model: $\hat{\eta} = \hat{\beta}_0 + \sum \hat{\beta}_i x_i$
- Contours of x_i and x_j are series of parallel lines
- Move in direction which increase $\hat{\eta}$ the quickest Move perpendicular to contour lines
- Direction based on slope estimates $\hat{\beta}_i$ and $\hat{\beta}_j$
- Often center points to make determination easier
- Choose step size for one of the variables (Δx_j)
- Move others accordingly (Table 11.3)

$$\Delta x_i = \frac{\hat{\beta}_i}{\hat{\beta}_j / \Delta x_j}$$

Example

Consider Problem 11.1 in Montgomery. A chemical plant produces oxygen by liquefying air and separating it into its component gases by fractional distillation. Current operating conditions are Temp = -220° C and pressure ratio of 1.2. Interested in maximizing the purity of oxygen.

```
temp = \frac{Temp + 220}{5} \qquad pres = \frac{Ratio - 1.2}{.1}
data purity;
input temp pres pure @@;
x1x1 = temp*temp;
x1x2 = temp*pres;
cards;
-1 -1 82.8 -1 1 83.5 1 -1 84.7 1 1 85.0
0 0 84.1 0 0 84.5 0 0 83.9 0 0 84.3
;
proc reg;
model pure = temp pres x1x1 x1x2; run;
```

Dependent Variable: PURE

| | | Sum of | Mean | | |
|---------|----|---------|---------|---------|--------|
| Source | DF | Squares | Square | F Value | Prob>F |
| Model | 4 | 3.26000 | 0.81500 | 12.225 | 0.0335 |
| Error | 3 | 0.20000 | 0.06667 | | |
| C Total | 7 | 3.46000 | | | |

Parameter Estimates

| | | Parameter | Standard | T for HO: | |
|----------|----|-----------|------------|-------------|-----------|
| Variable | DF | Estimate | Error | Parameter=0 | Prob > T |
| INTERCEP | 1 | 84.200000 | 0.12909944 | 652.210 | 0.0001 |
| TEMP | 1 | 0.850000 | 0.12909944 | 6.584 | 0.0071 |
| PRES | 1 | 0.250000 | 0.12909944 | 1.936 | 0.1482 |
| X1X1 | 1 | -0.200000 | 0.18257419 | -1.095 | 0.3534 |
| X1X2 | 1 | -0.100000 | 0.12909944 | -0.775 | 0.4950 |

A one degree change in temp is equivalent to a 1/5=.2 temp step once standardized. Thus means we increase pressure by (.2)(.25/.85) = .059. The following table summarizes moving in this direction and the observed purity (**simulated results**). It appears that a maximum is reached around ten steps. Another linear approximation should be made centered now at (-210,1.2590).

| | Coded | | Na | tural | |
|-------|-------|--------|------|--------|----------|
| | Var | iables | Vari | ables | |
| Steps | x_1 | x_2 | Temp | Pres | Response |
| 0 | 0.0 | 0.000 | -220 | 1.2 | 84.2 |
| 1 | 0.2 | 0.059 | -219 | 1.2059 | 84.7 |
| 5 | 1.0 | 0.295 | -215 | 1.2295 | 85.2 |
| 10 | 2.0 | 0.590 | -210 | 1.2590 | 85.3 |
| 15 | 3.0 | 0.885 | -205 | 1.2885 | 85.1 |
| 20 | 4.0 | 1.180 | -200 | 1.3180 | 84.7 |

 $\hat{y}_{ij} = 84.10 + .85x_T + .25x_P$

Checking Linear Approximation

- Do Lack of Fit Test
 - Use the center points to estimate pure error. Use $SS_{Interaction}$ or $\hat{\beta}_{12}$ (created by adding x_1x_2 term in the model) to compute lack of fit error.

$$\hat{\sigma}^2 = (84.1^2 + \dots + 84.3^2 - 336.8^2/4)/3 = .2/3 = .0666$$

– If linear, there will be no interaction effect. $\hat{\beta}_{12}$ is simply half the estimated effect,

$$2\hat{\beta}_{12} = .5(82.8 + 85.0 - 83.5 - 84.7) = -.2$$

- The SS₁₂= $(-.4)^2/4 = .04$. This is also the lack-of-fit SS. The F test is .04/.0666 = 0.6 and has a P-value of around .5.
- Compare average of center points to design points
 - If there is no curvature, the average of the four design points should be equal to the average of the center points. The difference between these two averages is an estimate of the pure quadratic term $\beta_{11} + \beta_{22}$. In this example, it is 336/4 336.8/4 = -.2.
 - The SS is $(4)(4)(-.2)^2/(4+4) = .08$. The F test is .08/.06666 = 1.33 and has a P-value of around .3. This also suggests that the linear model is appropriate.

Analysis of Second Order Model

• Due to curvature, determine **stationary point**

$$\frac{\partial \hat{\eta}}{\partial x_i} = 0$$

- Stationary point may be minimum, maximum, or saddle point
- Use contours or canonical analysis to determine behavior
- Can write quadratic approximation as (page 440)

$$y = \beta_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x} + \epsilon$$

- Solution is $\mathbf{x}_s = -.5\mathbf{B}^{-1}\mathbf{b}$
- ullet Canonical analysis looks at eigenvalues and eigenvectors of f B

Example

Consider Problem 11.8 in Montgomery. An experimenter wants to optimize crystal growth as a function of three variables x_1, x_2 , and x_3 . The design used is a factorial with six center points and six axial points (see Figure 11-20). We will use Proc RSREG which does a quadratic response surface analysis.

```
data purity;
```

| İ | Input | 2 2 | x1 x2 | 2 x3 | re | esp | @@; | С | arc | ls; | | | | | | |
|----|-------|-----|-------|-------|----|-----|-----|-----|-----|-----|-----|----|------|-----|-----|-----|
| -1 | - | -1 | -1 | 6 | 6 | -1 | | -1 | 1 | | 70 | -1 | | 1 | -1 | 78 |
| -1 | | 1 | 1 | 6 | 0 | 1 | | -1 | -1 | | 80 | 1 | - | -1 | 1 | 70 |
| 1 | | 1 | -1 | 10 | 0 | 1 | | 1 | 1 | | 75 | -1 | .682 | 0 | 0 | 100 |
| 1. | .682 | 0 | 0 | 8 | 0 | 0 | -1. | 682 | 2 0 | | 68 | 0 | 1. | 682 | 2 0 | 63 |
| 0 | | 0 | -1.0 | 682 6 | 5 | 0 | | 0 | 1. | 682 | 82 | 0 | | 0 | 0 | 113 |
| 0 | 0 | | 0 | 10 | 0 | 0 | | 0 | 0 | - | L18 | 0 | | 0 | 0 | 88 |
| 0 | 0 | | 0 | 10 | 0 | 0 | | 0 | 0 | | 85 | | | | | |
| ; | | | | | | | | | | | | | | | | |

proc rsreg;

model resp=x1 x2 x3 / lackfit; run;

Breaks Down Regression SS into Linear, Quadratic Terms

| | Degrees | | | | |
|---------------|---------|-------------|----------|---------|----------|
| | of | Type I Sum | | | |
| Regression | Freedom | of Squares | R-Square | F-Ratio | Prob > F |
| Linear | 3 | 77.854973 | 0.0141 | 0.139 | 0.9341 |
| Quadratic | 3 | 3291.741253 | 0.5960 | 5.896 | 0.0139 |
| Crossproduct | 3 | 292.375000 | 0.0529 | 0.524 | 0.6757 |
| Total Regress | 9 | 3661.971227 | 0.6630 | 2.186 | 0.1194 |

**Appears to be a quadratic component but very little crossproduct **Overall regression not significant but that's not concern **Would expect contours to be fairly circular

Does Lack of Fit Test

| | Degrees | | | | |
|-------------|---------|-------------|-------------|---------|----------|
| | of | Sum of | | | |
| Residual | Freedom | Squares | Mean Square | F-Ratio | Prob > F |
| Lack of Fit | 5 | 1001.645440 | 200.329088 | 1.166 | 0.4353 |
| Pure Error | 5 | 859.333333 | 171.866667 | | |
| Total Error | 10 | 1860.978773 | 186.097877 | | |

**No apparent lack of fit to quadratic model

Gives the Parameter Estimates and Standard Errors

| | Deg of | Parameter | Standard | T for HO: |
|-----------|---------|------------|----------|-------------|
| Parameter | Freedom | Estimate | Error | Parameter=0 |
| INTERCEPT | 1 | 100.666301 | 5.563818 | 18.093 |
| X1 | 1 | 1.271027 | 3.691248 | 0.344 |
| X2 | 1 | 1.361082 | 3.691248 | 0.369 |
| ХЗ | 1 | -1.494042 | 3.691248 | -0.405 |
| X1*X1 | 1 | -3.767908 | 3.592852 | -1.049 |
| X2*X1 | 1 | 2.875000 | 4.823094 | 0.596 |
| X2*X2 | 1 | -12.427833 | 3.592852 | -3.459 |
| X3*X1 | 1 | -2.625000 | 4.823094 | -0.544 |
| X3*X2 | 1 | -4.625000 | 4.823094 | -0.959 |
| X3*X3 | 1 | -9.600102 | 3.592852 | -2.672 |

Performs Canonical Analysis

| | Degrees | | | | |
|--------|---------|-------------|-------------|---------|----------|
| | of | Sum of | | | |
| Factor | Freedom | Squares | Mean Square | F-Ratio | Prob > F |
| X1 | 4 | 347.989342 | 86.997336 | 0.467 | 0.7587 |
| X2 | 4 | 2489.210554 | 622.302639 | 3.344 | 0.0553 |
| ХЗ | 4 | 1585.399212 | 396.349803 | 2.130 | 0.1515 |

Canonical Analysis of Response Surface (based on coded data)

Critical Value

| Factor | Coded | Uncoded |
|--------|-----------|-----------|
| X1 | 0.154420 | 0.259735 |
| X2 | 0.065908 | 0.110858 |
| ХЗ | -0.083251 | -0.140028 |

Predicted value at stationary point 101.011413

Eigenvectors

| Eigenvalues | Xl | X2 | ХЗ |
|-------------|-----------|-----------|-----------|
| -8.711273 | 0.941384 | 0.210046 | -0.263964 |
| -25.327160 | 0.330987 | -0.424011 | 0.843008 |
| -38.941204 | -0.065147 | 0.880963 | 0.468679 |

Stationary point is a maximum.

Response Surface Designs

- Want points sparse but give info over entire region
- Blocking is possible
- Designs can be built sequentially
- Provides internal estimate of error/lack of fit
- Orthogonal first order designs
 - Minimize the variance of regression coefficients
 - -2^k Factorial (with center points)
 - Fractional factorial of resolution III or higher
- Central composite designs (2nd order)
 - -2^k factorial
 - Fractional factorial of resolution V or higher
 - Add center points and 2k axial runs