Assignment 4 – STAT453/558 Spring 2024
Due date April 2nd,2024

Question 1 - The data shown in the table below were collected in an experiment to optimize crystal growth as a function of three variables x_1, x_2, and x_3. Large values of y (yield in grams) are desirable. Fit a second order model and analyze the fitted surface. Under what set of conditions is maximum growth achieved?

x_1	x_2	x_3	y
-1	-1	-1	66
-1	-1	1	70
-1	1	-1	78
-1	1	1	60
1	-1	-1	80
1	-1	1	70
1	1	-1	100
1	1	1	75
-1.682	0	0	100
1.682	0	0	80
0	-1.682	0	68
0	1.682	0	63
0	0	-1.682	65
0	0	1.682	82
0	0	0	113
0	0	0	100
0	0	0	118
0	0	0	88
0	0	0	100
0	0	0	85

```r
library(rsm)

# Create a data frame with the provided data
data <- data.frame(
  x1 = c(-1, -1, -1, -1, 1, 1, 1, 1, -1.682, 1.682, 0, 0, 0, 0, 0, 0, 0, 0, 0,0),
  x2 = c(-1, -1, 1, 1, -1, -1, 1, 1, 0, 0, -1.682, 1.682, 0, 0, 0, 0, 0, 0, 0, 0),
  x3 = c(-1, 1, -1, 1, -1, 1, -1, 1, 0, 0, 0, 0, -1.682, 1.682, 0, 0, 0, 0, 0, 0),
  y = c(66, 70, 78, 60, 80, 70, 100, 75, 100, 80, 68, 63, 65, 82, 113, 100, 118, 88, 100, 85)
)

# Load the rsm package
library(rsm)



# Fit the response surface model to the data
model <- rsm(y ~ SO(x1, x2, x3)^2, data = data)

# Print the model summary
summary(model)
```

```
##
## Call:
## rsm(formula = y ~ SO(x1, x2, x3)^2, data = data)
##
##             Estimate Std. Error t value  Pr(>|t|)
## (Intercept) 100.6663     5.5638 18.0930 5.703e-09 ***
## x1            1.2710     3.6912  0.3443  0.737726
## x2            1.3611     3.6912  0.3687  0.720014
## x3           -1.4940     3.6912 -0.4048  0.694182
## x1:x2         2.8750     4.8231  0.5961  0.564363
## x1:x3        -2.6250     4.8231 -0.5443  0.598190
## x2:x3        -4.6250     4.8231 -0.9589  0.360205
## x1^2         -3.7679     3.5929 -1.0487  0.318990
## x2^2        -12.4278     3.5929 -3.4590  0.006133 **
## x3^2         -9.6001     3.5929 -2.6720  0.023412 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Multiple R-squared:  0.663,  Adjusted R-squared:  0.3598
## F-statistic: 2.186 on 9 and 10 DF,  p-value: 0.1194
##
## Analysis of Variance Table
##
## Response: y
##                 Df Sum Sq Mean Sq F value Pr(>F)
## FO(x1, x2, x3)   3   77.9   25.95  0.1395 0.9341
## TWI(x1, x2, x3)  3  292.4   97.46  0.5237 0.6757
## PQ(x1, x2, x3)   3 3291.7 1097.25  5.8961 0.0139
## Residuals       10 1861.0  186.10
## Lack of fit      5 1001.6  200.33  1.1656 0.4353
## Pure error       5  859.3  171.87
##
## Stationary point of response surface:
##         x1        x2         x3
##  0.2597353 0.1108581 -0.1400280
##
## Eigenanalysis:
## eigen() decomposition
```

```
## $values
## [1]  -3.079142  -8.952298 -13.764404
##
## $vectors
##            [,1]       [,2]        [,3]
## x1  0.9413839  0.3309866 -0.06514712
## x2  0.2100461 -0.4240105  0.88096295
## x3 -0.2639639  0.8430083  0.46867915
```

```
# Plot the fitted surface
contour(model, ~x1 + x2, interactive = TRUE)
```

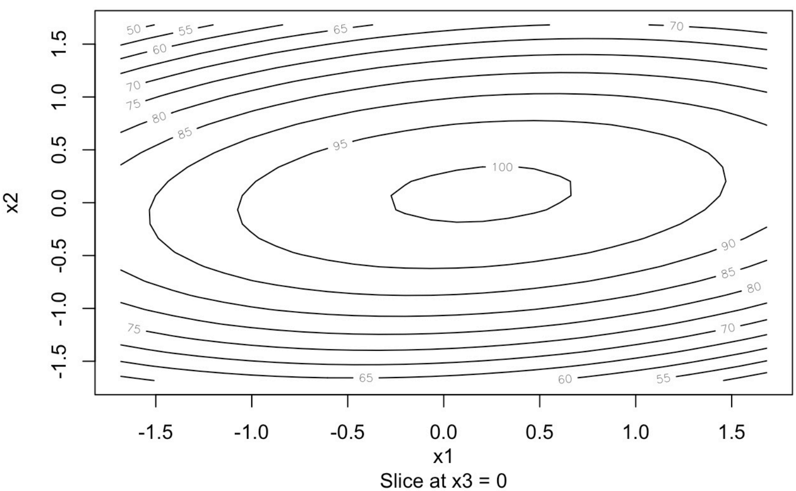
```
## Warning in plot.window(xlim, ylim, ...): "interactive" is not a graphical
## parameter
```

```
## Warning in title(...): "interactive" is not a graphical parameter
```

```
## Warning in axis(side = side, at = at, labels = labels, ...): "interactive" is
## not a graphical parameter

## Warning in axis(side = side, at = at, labels = labels, ...): "interactive" is
## not a graphical parameter
```

```
## Warning in box(...): "interactive" is not a graphical parameter
```




```
#To find the conditions for maximum growth,
#I need to check he stationary point of the response surface. The stationary point is where the gradient of the r
esponse surface is zero, indicating a potential maximum or minimum.

#According to the model summary, the stationary point is at:
#x1 =  0.2597353 x2 = 0.1108581 x3 = -0.1400280

#Therefore, under the conditions where x1 is approximately 0.2597, x2 is approximately 0.1109, and x3 is approxim
ately -0.1400, the maximum growth is achieved.
```

Question 2 - An experimenter has run a Box-Behnken design and has obtained the results as shown in the table below, where the response variable is the viscosity of a polymer.

Level	Temp.	Agitation Rate	Pressure	x_1	x_2	x_3
High	200	10.0	25	+1	+1	+1
Middle	175	7.5	20	0	0	0
Low	150	5.0	15	-1	-1	-1

Run	x_1	x_2	x_3	y_1
1	-1	-1	0	535
2	1	-1	0	580
3	-1	1	0	596
4	1	1	0	563
5	-1	0	-1	645
6	1	0	-1	458
7	-1	0	1	350
8	1	0	1	600
9	0	-1	-1	595
10	0	1	-1	648
11	0	-1	1	532
12	0	1	1	656
13	0	0	0	653
14	0	0	0	599
15	0	0	0	620

(a) Fit the second-order model.

(b) Perform the canonical analysis. What type of surface has been found?

(c) What operating conditions on x_1, x_2, and x_3 maximize viscosity?

```r
# Load the rsm package
library(rsm)

# Create a data frame with the provided data
data <- data.frame(
  x1 = c(-1, 1, -1, 1, -1, 1, -1, 1, 0, 0, 0, 0, 0, 0, 0),
  x2 = c(-1, -1, 1, 1, 0, 0, 0, 0, -1, 1, -1, 1, 0, 0, 0),
  x3 = c(0, 0, 0, 0, -1, -1, 1, 1, -1, -1, 1, 1, 0, 0, 0),
  y = c(535, 580, 596, 563, 645, 458, 350, 600, 595, 648, 532, 656, 653, 599, 620)
)

# Fit the second-order model to the data
model <- rsm(y ~ SO(x1, x2, x3)^2, data = data)


# Print the model summary
summary(model)
```

```
##
## Call:
## rsm(formula = y ~ SO(x1, x2, x3)^2, data = data)
##
##             Estimate Std. Error t value  Pr(>|t|)
## (Intercept)  624.000     18.652 33.4539 4.487e-07 ***
## x1             9.375     11.422  0.8208  0.449128
## x2            27.625     11.422  2.4185  0.060228 .
## x3           -26.000     11.422 -2.2763  0.071874 .
## x1:x2        -19.500     16.154 -1.2072  0.281356
## x1:x3        109.250     16.154  6.7632  0.001074 **
## x2:x3         17.750     16.154  1.0988  0.321915
## x1^2         -75.000     16.813 -4.4608  0.006636 **
## x2^2          19.500     16.813  1.1598  0.298496
## x3^2         -35.750     16.813 -2.1263  0.086809 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## Multiple R-squared:  0.945,  Adjusted R-squared:  0.846
## F-statistic: 9.544 on 9 and 5 DF,  p-value: 0.0115
##
## Analysis of Variance Table
##
## Response: y
##                  Df Sum Sq Mean Sq F value   Pr(>F)
## FO(x1, x2, x3)    3  12216  4072.1  3.9014 0.088473
## TWI(x1, x2, x3)   3  50524 16841.2 16.1352 0.005278
## PQ(x1, x2, x3)    3  26913  8970.9  8.5949 0.020359
## Residuals         5   5219  1043.7
## Lack of fit       3   3737  1245.6  1.6809 0.394113
## Pure error        2   1482   741.0
##
## Stationary point of response surface:
##         x1         x2         x3
##  2.1849596 -0.8713709  2.7586015
##
## Eigenanalysis:
## eigen() decomposition
## $values
## [1]   20.922869    2.520763 -114.693632
##
## $vectors
##           [,1]       [,2]       [,3]
## x1 -0.02739155  0.5811826  0.8133121
## x2  0.99128775 -0.0890686  0.0970329
## x3  0.12883440  0.8088842 -0.5736794
```

```
#b

#To determine the type of surface found we can analyze the coefficients.


#If all linear coefficients (x1, x2, x3) are positive and all interaction coefficients are negative, it indicates a ridge.
#If all linear coefficients are negative and all interaction coefficients are positive, it indicates a valley.
#If the signs are mixed, it indicates a saddle point.

#Igot x1: 9.375 x2: 27.625 x3: -26.000

#The interaction coefficients are:
#x1:x2: -19.500 x1:x3: 109.250 x2:x3: 17.750
#We can see that the linear coefficients are not all positive or all negative, and the interaction coefficients are not all negative or all positive. Therefore, the type of surface that has been found is likely a saddle point.









#c
# Perform steepest ascent analysis
steepest(model)
```

```
## Path of steepest ascent from ridge analysis:
```

```
##    dist     x1    x2     x3 |     yhat
## 1   0.0  0.000 0.000  0.000 |  624.000
## 2   0.5 -0.066 0.472 -0.150 |  643.966
## 3   1.0 -0.127 0.979 -0.162 |  672.465
## 4   1.5 -0.166 1.484 -0.137 |  710.887
## 5   2.0 -0.196 1.988 -0.096 |  759.699
## 6   2.5 -0.220 2.490 -0.048 |  818.876
## 7   3.0 -0.242 2.990  0.005 |  888.382
## 8   3.5 -0.262 3.490  0.061 |  968.463
## 9   4.0 -0.280 3.988  0.119 | 1058.752
## 10  4.5 -0.298 4.487  0.178 | 1159.791
## 11  5.0 -0.314 4.984  0.238 | 1270.924
```

```
# Based on the output I got, the operating conditions that maximize viscosity are approximately:
#x1 = -0.314 x2 = 4.984 x3 = 0.238

#Therefore, to maximize viscosity, I need to use
#x1 = -0.314 x2 = 4.984 x3 = 0.238
```