Residual Surface Methodology

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CODING OF DATA

We begin by first installing rsm package (if not installed) and load it.

```
#Install and load package
#install.packages("rsm")
library(rsm)
```

```
## Warning: package 'rsm' was built under R version 4.3.2
```

The package contains a data set called ChemReact1, load and view the sample data.

```
ChemReact1
```

```
##   Time Temp Yield
## 1   80  170  80.5
## 2   80  180  81.5
## 3   90  170  82.0
## 4   90  180  83.5
## 5   85  175  83.9
## 6   85  175  84.3
## 7   85  175  84.0
```

This dataframe contains the variables Time and Temperature are continuous independent variables and Yield is a continuous dependent variable.

We will use coded.data to code them as x1 and x2, respectively:

```
#name of the coded variable ~ linear expression fir the uncoded variable
CR1 <- coded.data(ChemReact1, x1 ~ (Time - 85)/5,
                  x2 ~ (Temp - 175)/5)
CR1
```

```
##   Time Temp Yield
## 1   80  170  80.5
## 2   80  180  81.5
## 3   90  170  82.0
## 4   90  180  83.5
## 5   85  175  83.9
## 6   85  175  84.3
## 7   85  175  84.0
##
## Data are stored in coded form using these coding formulas ...
## x1 ~ (Time - 85)/5
## x2 ~ (Temp - 175)/5
```

The dataframe looks very similar to how they were presented in the original, ChemReact1 dataframe, but see they are internally Time and Temp are internally understood by R as x1 and x2. This can be witnessed if CR1 is coerced into a standard dataframe:

```
as.data.frame(CR1)
```

```
##   x1 x2 Yield
## 1 -1 -1  80.5
## 2 -1  1  81.5
## 3  1 -1  82.0
## 4  1  1  83.5
## 5  0  0  83.9
## 6  0  0  84.3
## 7  0  0  84.0
```

This is important so that the dataframe is compatible with downstream rsm package functions.

Generating a design

Function for creating a Box-Behnken design - bbd

Function for creating a central composite design - ccd

Box-Behnken design

Create a 3-factor Box-Behnken design with two center points:

```
bbd(3, n0 = 2, coding =list(x1 ~ (Force - 20)/3, x2 ~ (Rate - 50)/10, x3 ~ Polish - 4))
```

```
##    run.order std.order Force Rate Polish
## 1          1         5    17   50      3
## 2          2         6    23   50      3
## 3          3        12    20   60      5
## 4          4         4    23   60      4
## 5          5         1    17   40      4
## 6          6         8    23   50      5
## 7          7         2    23   40      4
## 8          8         3    17   60      4
## 9          9        11    20   40      5
## 10        10         7    17   50      5
## 11        11        10    20   60      3
## 12        12         9    20   40      3
## 13        13        13    20   50      4
## 14        14        14    20   50      4
##
## Data are stored in coded form using these coding formulas ...
## x1 ~ (Force - 20)/3
## x2 ~ (Rate - 50)/10
## x3 ~ Polish - 4
```

This example of an experiment has 3 variables (x1, x2, and x3). The experiment is randomized.

If there were a 4th or 5th variable, then the design would be blocked (default setting) and the blocks would be individually randomized

Central composite design

CCD is a popular design because it allows the experimenter to iterizatively improve a system through optimization experiments

One could first experiment with a single block for a first-order model and then add more block(s) if necessray to perform a second-order model fit

There are two types of CCD blocks

- Cube block - has design points from a two-level factorial or fractional factorial design plus center points

  -best predictions are found within the confines of these points

  -Used to estimate main effects and two factor interactions

- Star block - contains axis points and center points

  -Used to estimate quadratic effects

FITTING A RESPONSE SURFACE MODEL

The rsm function must make use of the following arguments:

- FO() - first order
- TWI() - two-way intereaction
- PQ() - pure quadratic
- SO() - second order

Fit first order response-surface model to the data in the first block;

```
CR1.rsm <- rsm(Yield ~ FO(x1, x2), data = CR1)
summary(CR1.rsm)
```

```
##
## Call:
## rsm(formula = Yield ~ FO(x1, x2), data = CR1)
##
##             Estimate Std. Error  t value  Pr(>|t|)
## (Intercept) 82.81429    0.54719 151.3456 1.143e-08 ***
## x1           0.87500    0.72386   1.2088    0.2933
## x2           0.62500    0.72386   0.8634    0.4366
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Multiple R-squared:  0.3555, Adjusted R-squared:  0.0333
## F-statistic: 1.103 on 2 and 4 DF,  p-value: 0.4153
##
## Analysis of Variance Table
##
## Response: Yield
##             Df Sum Sq Mean Sq F value  Pr(>F)
## FO(x1, x2)   2 4.6250  2.3125  1.1033 0.41534
## Residuals    4 8.3836  2.0959
## Lack of fit  2 8.2969  4.1485 95.7335 0.01034
## Pure error   2 0.0867  0.0433
##
## Direction of steepest ascent (at radius 1):
```

```
##        x1        x2
## 0.8137335 0.5812382
##
## Corresponding increment in original units:
##     Time     Temp
## 4.068667 2.906191
```

- The summary of this model indicates that there is a significant lack of fit ($p = 0.01034$)
- This suggests that it may be a good idea to test a higher order model

Model with two-way interactions:

```
CR1.rsmi <- update(CR1.rsm, . ~ . + TWI(x1, x2))
summary(CR1.rsmi)
```

```
##
## Call:
## rsm(formula = Yield ~ FO(x1, x2) + TWI(x1, x2), data = CR1)
##
##             Estimate Std. Error  t value  Pr(>|t|)
## (Intercept) 82.81429    0.62948 131.5604 9.683e-07 ***
## x1           0.87500    0.83272   1.0508    0.3705
## x2           0.62500    0.83272   0.7506    0.5074
## x1:x2        0.12500    0.83272   0.1501    0.8902
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Multiple R-squared:  0.3603, Adjusted R-squared:  -0.2793
## F-statistic: 0.5633 on 3 and 3 DF,  p-value: 0.6755
##
## Analysis of Variance Table
##
## Response: Yield
##             Df Sum Sq Mean Sq  F value   Pr(>F)
## FO(x1, x2)   2 4.6250  2.3125   0.8337 0.515302
## TWI(x1, x2)  1 0.0625  0.0625   0.0225 0.890202
## Residuals    3 8.3211  2.7737
## Lack of fit  1 8.2344  8.2344 190.0247 0.005221
## Pure error   2 0.0867  0.0433
##
## Stationary point of response surface:
## x1 x2
## -5 -7
##
## Stationary point in original units:
## Time Temp
##   60  140
##
## Eigenanalysis:
## eigen() decomposition
## $values
## [1]  0.0625 -0.0625
##
## $vectors
##         [,1]       [,2]
```

```
## x1 0.7071068 -0.7071068
## x2 0.7071068  0.7071068
```

The p-value for the lack of fit test is still very small (p = 0.005221). To investigate further, more data is needed so we can combine two blocks of the greater ChemReact experiment (ChemReact1 + ChemReact2):

```
(CR2 <- djoin(CR1, ChemReact2))
```

```
##     Time   Temp Yield Block
## 1  80.00 170.00  80.5     1
## 2  80.00 180.00  81.5     1
## 3  90.00 170.00  82.0     1
## 4  90.00 180.00  83.5     1
## 5  85.00 175.00  83.9     1
## 6  85.00 175.00  84.3     1
## 7  85.00 175.00  84.0     1
## 8  85.00 175.00  79.7     2
## 9  85.00 175.00  79.8     2
## 10 85.00 175.00  79.5     2
## 11 92.07 175.00  78.4     2
## 12 77.93 175.00  75.6     2
## 13 85.00 182.07  78.5     2
## 14 85.00 167.93  77.0     2
##
## Data are stored in coded form using these coding formulas ...
## x1 ~ (Time - 85)/5
## x2 ~ (Temp - 175)/5
```

The larger dataset allows us to fit a full second-order model to the data. This can be accomplished by using the following code:

```
CR2.rsm <- rsm(Yield ~ Block + SO(x1, x2), data = CR2)
summary(CR2.rsm)
```

```
##
## Call:
## rsm(formula = Yield ~ Block + SO(x1, x2), data = CR2)
##
##              Estimate Std. Error  t value  Pr(>|t|)
## (Intercept) 84.095427   0.079631 1056.067 < 2.2e-16 ***
## Block2      -4.457530   0.087226  -51.103 2.877e-10 ***
## x1           0.932541   0.057699   16.162 8.444e-07 ***
## x2           0.577712   0.057699   10.012 2.122e-05 ***
## x1:x2        0.125000   0.081592    1.532    0.1694
## x1^2        -1.308555   0.060064  -21.786 1.083e-07 ***
## x2^2        -0.933442   0.060064  -15.541 1.104e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Multiple R-squared:  0.9981, Adjusted R-squared:  0.9964
## F-statistic: 607.2 on 6 and 7 DF,  p-value: 3.811e-09
##
## Analysis of Variance Table
##
## Response: Yield
##             Df Sum Sq Mean Sq   F value    Pr(>F)
```

```
## Block        1 69.531  69.531 2611.0950 2.879e-10
## FO(x1, x2)   2  9.626   4.813  180.7341 9.450e-07
## TWI(x1, x2)  1  0.063   0.063    2.3470    0.1694
## PQ(x1, x2)   2 17.791   8.896  334.0539 1.135e-07
## Residuals    7  0.186   0.027
## Lack of fit  3  0.053   0.018    0.5307    0.6851
## Pure error   4  0.133   0.033
##
## Stationary point of response surface:
##        x1        x2
## 0.3722954 0.3343802
##
## Stationary point in original units:
##      Time      Temp
##  86.86148 176.67190
##
## Eigenanalysis:
## eigen() decomposition
## $values
## [1] -0.9233027 -1.3186949
##
## $vectors
##          [,1]       [,2]
## x1 -0.1601375 -0.9870947
## x2 -0.9870947  0.1601375
```

- In this model, the lack of fit is not significant (p = 0.6851)
- The stationary point values are like the coordinates for the center of the plot
- In the Eigen analysis, both eigenvalues are negative

This is indicative that the stationary point is a maximum

This is an ideal situation in which the optimal conditions for this system are in close range of the stationary point

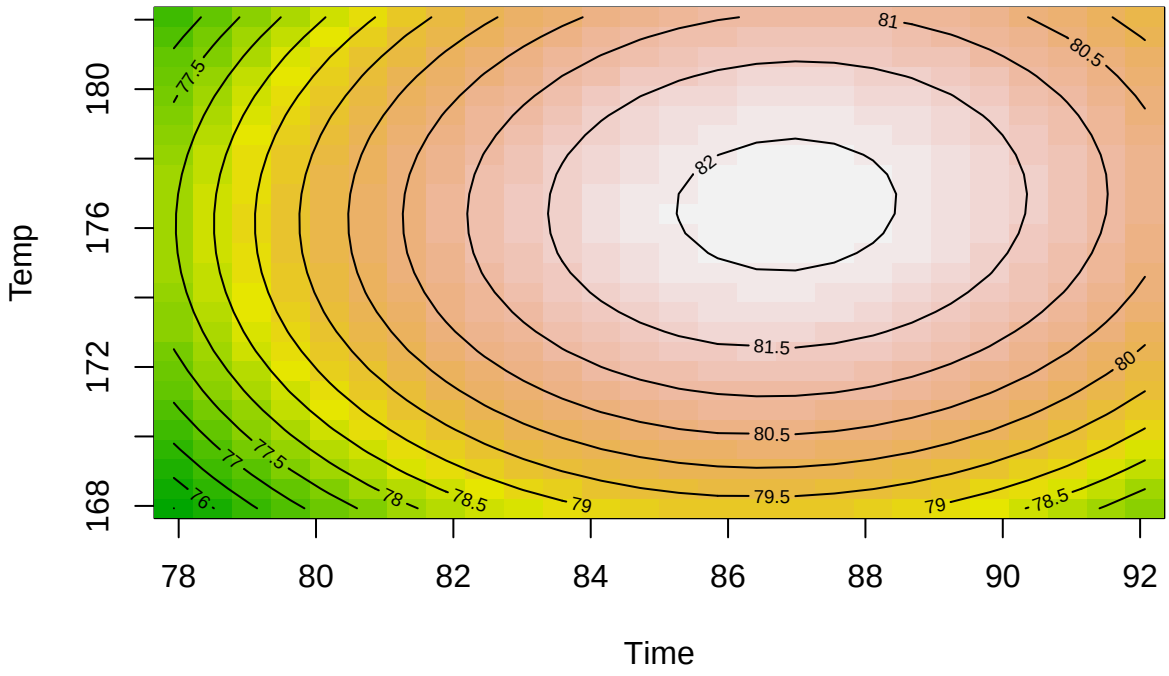
The next step would be to collect more data around this estimated optimum point when

Time = 86.86148 min

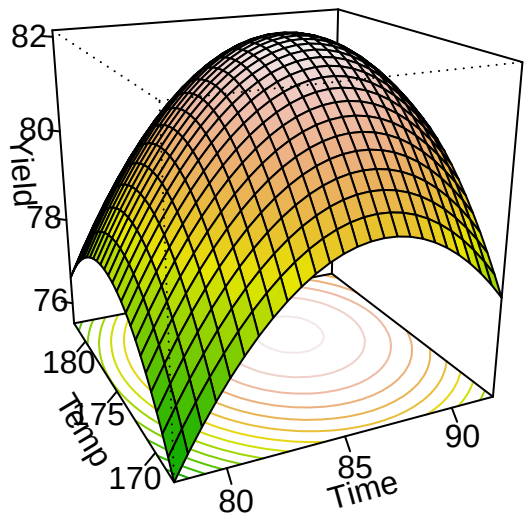
Temp = 176.67190 C

Visualization with a contour and perspective plot

```
#par(mfrow = c(1,1))
contour(CR2.rsm, ~ x1 + x2, image = TRUE, at = summary(
  CR2.rsm)$canonical$xs)
```




```
persp(CR2.rsm, x2 ~ x1, col = terrain.colors(50),
      contours = 'colors', zlab = "Yield", main="Second-order model")
```



Direction for further experimentation

- In many first-order and some second-order cases, we find that the saddle point or stationary point is far from the optimal experimental region
- If this is the case then the most practical the next is to determine where in which direction to investigate further
- This is a facet of RSM called direction of steepest ascent

The rsm summary table provides information about this concept and we can zoom into that using the steepest function:

```
#dataframe to access and distance
steepest(CR1.rsm,dist = c(0,0.5,1))
```

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

```
##   dist    x1    x2 |   Time    Temp |   yhat
## 1  0.0 0.000 0.000 | 85.000 175.000 | 82.814
## 2  0.5 0.407 0.291 | 87.035 176.455 | 83.352
## 3  1.0 0.814 0.581 | 89.070 177.905 | 83.890
```

- yhat is the predicted value of the response variable in the model
- any set of distances can be factored in using the dist argument
- However, while the fitted values are displayed, remember that these are only predictions
- As the distance along the path increases, the predictions become less reliable

- The real use case of the path of steepest ascent is to determine the next set of experiments to get close to the optimal experimental conditions
- For a second-order model, the steepest function works, but it employs the 'ridge analysis method' which is a type of analog of the steepest ascent
- In this method, for a specified distance, d, a point at which the predicted response is a maximum among all predictor combinations at radius d can be determined
- It is sensible to use this method when the stationary point is somewhat far away