Ch-06 R Codes

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Textbook: Montgomery, D. C. (2012). *Design and analysis of experiments*, 8th Edition. John Wiley & Sons.

Online handouts: https://github.com/PingYangChen/ANOVA_Course_R_Code

2^2-Design: Chemical Process Example

Read the csv file `6_ChemicalRecovery.csv` in R.

```
df5 <- read.csv(file.path("data", "6_ChemicalRecovery.csv"))
```

The estimation of factor effects are:

```
# Effect of factor A (reactant concentration)
mean(df5$Recovery[df5$ReactConc == 1] - df5$Recovery[df5$ReactConc == -1])
# or 2*mean(df5$Recovery*df5$ReactConc)

# Effect of factor A (catalyst amount)
mean(df5$Recovery[df5$CataAmo == 1] - df5$Recovery[df5$CataAmo == -1])

# Effect of two-factor interaction AB
twofi <- as.numeric(df5$ReactConc)*df5$CataAmo
mean(df5$Recovery[twofi == 1] - df5$Recovery[twofi == -1])
```

```
## Effect of factor A (reactant concentration): 8.3333
```

```
## Effect of factor A (catalyst amount): -5.0000
```

```
## Effect of two-factor interaction AB: 1.6667
```

Use `aov()` to fit the ANOVA model (model description in math is omitted). Here, if the columns of the factor in the `data.frame` are not of the `factor` type. We can also specify the type of the factors as `factor` in the R model formula.

```
fit5 <- aov(Recovery ~ factor(ReactConc)*factor(CataAmo), data = df5)
summary(fit5)
```

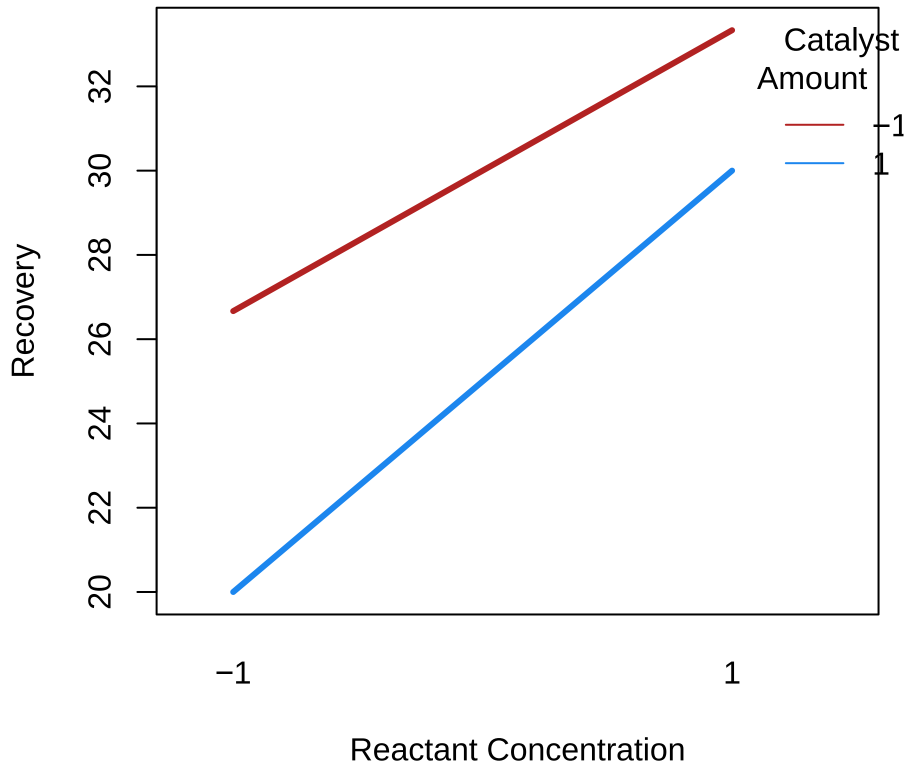
```
##                                   Df Sum Sq Mean Sq F value   Pr(>F)
## factor(ReactConc)                  1 208.33  208.33  53.191 8.44e-05 ***
## factor(CataAmo)                    1  75.00   75.00  19.149  0.00236 **
## factor(ReactConc):factor(CataAmo)  1   8.33    8.33   2.128  0.18278
## Residuals                          8  31.33    3.92
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The two main effects are significant and their two-factor interaction may not exist.

To visualize the analysis result of the factorial experiment, interaction plot is commonly used tool.

```
interaction.plot(
  x.factor = df5$ReactConc, # x-axis variable
```

```r
  trace.factor = df5$CataAmo, # variable for lines
  response = df5$Recovery, # y-axis variable
  ylab = "Recovery", xlab = "Reactant Concentration",
  col = c("firebrick", "dodgerblue2"),
  lty = 1, lwd = 3, trace.label = "Catalyst\nAmount"
)
```



2^3-Design: Plasma Etching Example

Read the csv file `6_PlasmaEtching_2^3.csv` in R.

```r
df6 <- read.csv(file.path("data", "6_PlasmaEtching_2^3.csv"))
```

The estimation of factor effects are:

```r
# Effect of main effects
2*mean(df6$EachRate*df6$Gap)
2*mean(df6$EachRate*df6$GasFlow)
2*mean(df6$EachRate*df6$Power)

# Effect of two-factor interactions
GapGasFlow <- df6$Gap * df6$GasFlow
GapPower <- df6$Gap * df6$Power
GasFlowPower <- df6$GasFlow * df6$Power
2*mean(df6$EachRate*GapGasFlow)
2*mean(df6$EachRate*GapPower)
2*mean(df6$EachRate*GasFlowPower)

# Effect of three-factor interaction
GapGasFlowPower <- df6$Gap * df6$GasFlow * df6$Power
```

```r
2*mean(df6$EachRate*GapGasFlowPower)
```

```
##   Factor Est.Effect
## 1      A   -101.625
## 2      B      7.375
## 3      C    306.125
## 4     AB    -24.875
## 5     AC   -153.625
## 6     BC     -2.125
## 7    ABC      5.625
```

Use `aov()` to fit the ANOVA model (model description in math is omitted). Here, if the columns of the factor in the `data.frame` are not of the `factor` type. We can also specify the type of the factors as `factor` in the R model formula.

```r
fit6 <- aov(
  EachRate ~ factor(Gap) * factor(GasFlow) * factor(Power),
  data = df6
)
summary(fit6)
```

```
##                                           Df Sum Sq Mean Sq F value   Pr(>F)
## factor(Gap)                                1  41311   41311  18.339 0.002679
## factor(GasFlow)                            1    218     218   0.097 0.763911
## factor(Power)                              1 374850  374850 166.411 1.23e-06
## factor(Gap):factor(GasFlow)                1   2475    2475   1.099 0.325168
## factor(Gap):factor(Power)                  1  94403   94403  41.909 0.000193
## factor(GasFlow):factor(Power)              1     18      18   0.008 0.930849
## factor(Gap):factor(GasFlow):factor(Power)  1    127     127   0.056 0.818586
## Residuals                                  8  18020    2253
##
## factor(Gap)                               **
## factor(GasFlow)
## factor(Power)                             ***
## factor(Gap):factor(GasFlow)
## factor(Gap):factor(Power)                 ***
## factor(GasFlow):factor(Power)
## factor(Gap):factor(GasFlow):factor(Power)
## Residuals
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The significant effects are main effects `Gap` and `Power`, and, the two-factor interaction `Gap:Power`.

WE can also fit a response surface model and obtain the same conslusion.

```r
ols6_full <- lm(EachRate ~ Gap * GasFlow * Power, data = df6)
summary(ols6_full)
```

```
##
## Call:
## lm(formula = EachRate ~ Gap * GasFlow * Power, data = df6)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -65.50 -11.12   0.00  11.12  65.50
##
```

```
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)        776.062     11.865  65.406 3.32e-12 ***
## Gap                -50.812     11.865  -4.282 0.002679 **
## GasFlow              3.688     11.865   0.311 0.763911
## Power              153.062     11.865  12.900 1.23e-06 ***
## Gap:GasFlow        -12.438     11.865  -1.048 0.325168
## Gap:Power          -76.812     11.865  -6.474 0.000193 ***
## GasFlow:Power       -1.062     11.865  -0.090 0.930849
## Gap:GasFlow:Power    2.813     11.865   0.237 0.818586
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 47.46 on 8 degrees of freedom
## Multiple R-squared:  0.9661, Adjusted R-squared:  0.9364
## F-statistic: 32.56 on 7 and 8 DF,  p-value: 2.896e-05
```

The final RSM is the reduced model that those insignificant terms are removed from the full model. Now we can use the real value of the factot levels as the predictors' values fro this reduced model for better interpretation.

```r
ols6_reduced <- lm(EachRate ~ NumGap * NumPower, data = df6)
summary(ols6_reduced)
```

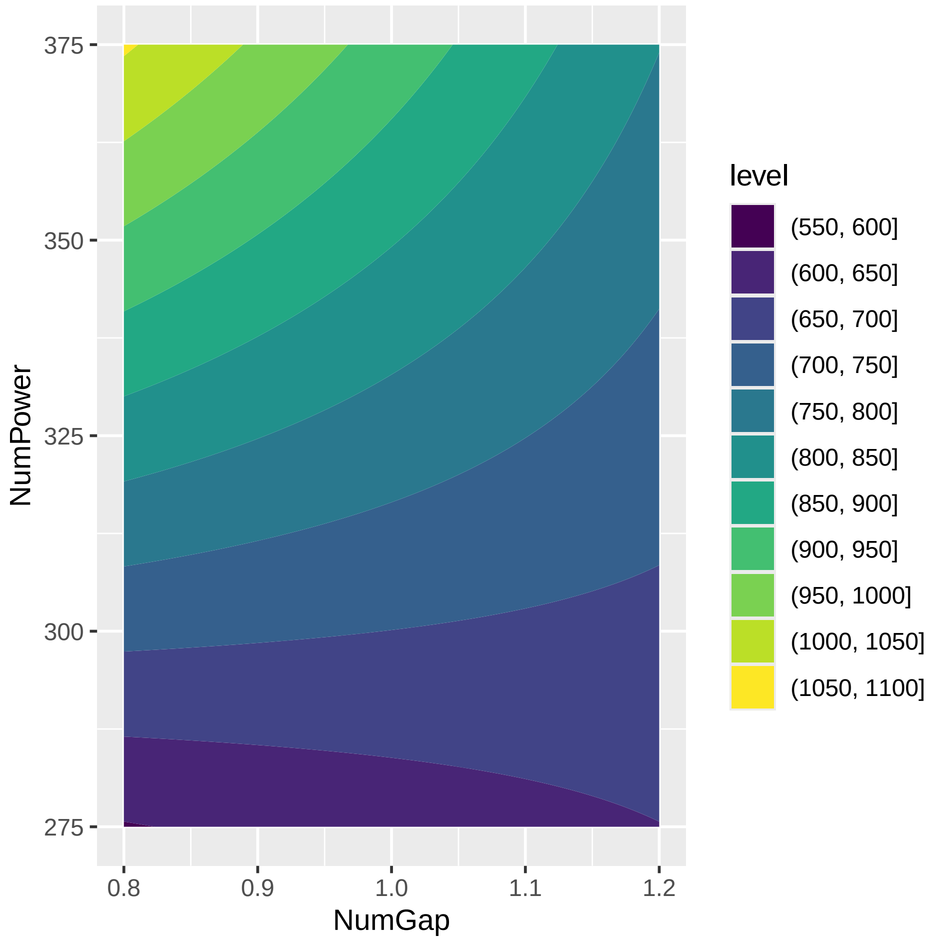
```
##
## Call:
## lm(formula = EachRate ~ NumGap * NumPower, data = df6)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -72.50 -15.44   2.50  18.69  66.50
##
## Coefficients:
##                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)     -2461.188    349.513  -7.042 1.35e-05 ***
## NumGap           2242.344    342.725   6.543 2.76e-05 ***
## NumPower           10.743      1.063  10.107 3.19e-07 ***
## NumGap:NumPower    -7.681      1.042  -7.370 8.62e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 41.69 on 12 degrees of freedom
## Multiple R-squared:  0.9608, Adjusted R-squared:  0.9509
## F-statistic: 97.91 on 3 and 12 DF,  p-value: 1.054e-08
```

```r
x1_grid <- seq(min(df6$NumGap), max(df6$NumGap), length = 100)
x2_grid <- seq(min(df6$NumPower), max(df6$NumPower), length = 100)
newx <- data.frame(
  NumGap = rep(x1_grid, each = 100),
  NumPower = rep(x2_grid, time = 100)
)

rsplot_data6 <- data.frame(newx, rs = predict(ols6_reduced, newx))

library(ggplot2)
#- Add color to the contour plot
```

```r
ggplot(rsplot_data6) +
  geom_contour(aes(NumGap, NumPower, z = rs), colour = "white") +
  geom_contour_filled(aes(NumGap, NumPower, z = rs))
```



Unreplicated 2^k Factorial Designs: The Resin Plant Experiment

Read the csv file `6_PilotPlant.csv` in R.

```r
df7 <- read.csv(file.path("data", "6_PilotPlant.csv"))
```

The estimation of factor effects are:

```r
# Compute the model matrix of all effect terms without intercept
mmat7 <- model.matrix( ~ Temperature*Pressure*CH2OConc*StirRate - 1, data = df7)
# Calculate the effect sizes using the +/- signs of the model matrix
eff7 <- numeric(ncol(mmat7))
for (i in 1:ncol(mmat7)) {
  eff7[i] <- 2*mean(df7$FiltrationRate*mmat7[,i])
}
names(eff7) <- colnames(mmat7)
```

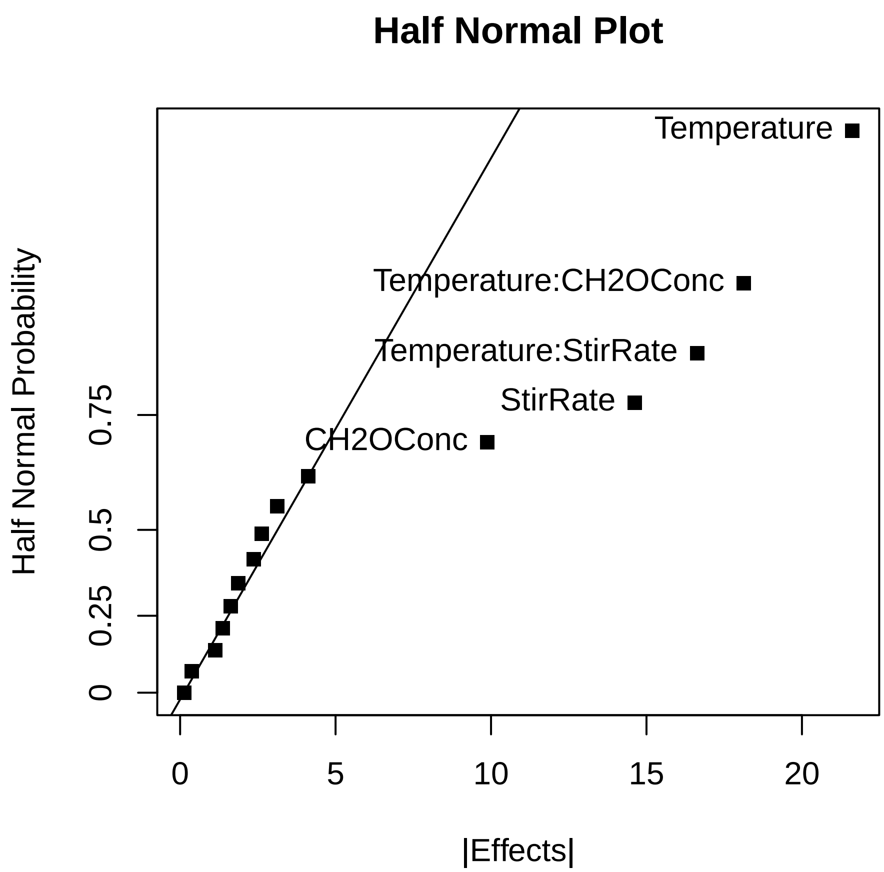
```
##                                     Factor Est.Effect
## 1                              Temperature     21.625
## 2                                 Pressure      3.125
## 3                                 CH2OConc      9.875
```

```
## 4                                      StirRate     14.625
## 5                          Temperature:Pressure      0.125
## 6                          Temperature:CH2OConc    -18.125
## 7                             Pressure:CH2OConc      2.375
## 8                          Temperature:StirRate     16.625
## 9                             Pressure:StirRate     -0.375
## 10                            CH2OConc:StirRate     -1.125
## 11            Temperature:Pressure:CH2OConc      1.875
## 12            Temperature:Pressure:StirRate      4.125
## 13            Temperature:CH2OConc:StirRate     -1.625
## 14               Pressure:CH2OConc:StirRate     -2.625
## 15 Temperature:Pressure:CH2OConc:StirRate      1.375
```

Because there is no replicates in each treatment combination, the estimate of the random error σ^2 does not exist and the ANOVA table is not available. Of all effect terms, we try of eliminate some of them before analyzing the data. According to the model assumption, the effects that are negligible should be similar to random error which is normally distributed with zero mean and constant variance. Therefore, a QQ-plot or half-Normal plot is helpful to identify effective effects. Belows are the codes of half-Normal plot.

```r
# Half Normal Plot
halfqqnorm <- function(input, tol = 0.5) {
    y <- sort(abs(input))
    nq <- qnorm(seq(0.5, 0.99, length = length(y)))
    plot(y, nq, yaxt = "n", pch = 15,
         xlab = "|Effects|", ylab = "Half Normal Probability")
    title("Half Normal Plot")
    # choose anchor point to draw a straight line
    s <- min(which(diff(y)/diff(range(y)) > 1/(length(y)-1)))
    abline(a = -y[1]*(nq[s]-nq[1])/(y[s]-y[1]), b = (nq[s]-nq[1])/(y[s]-y[1]))
    axis(2, at = qnorm(seq(0.5, 0.9999, length = 5)),
         labels = round(seq(0, 1, length = 5),2))
    loc <- sqrt((nq - (y - y[1])*(nq[s]-nq[1])/(y[s]-y[1]))^2) > tol
    if (is.null(names(y))) {
        text(y[loc], nq[loc], order(abs(input))[loc], pos = 2)
    } else {
        text(y[loc], nq[loc], names(abs(input))[order(abs(input))[loc]], pos = 2)
    }
}
```

```r
halfqqnorm(eff7)
```



By the half Normal plot, we find out that the main effects `Temperature`, `CH2OConc`and `StirRate` and interactions `Temperature:CH2OConc`, `Temperature:StirRate` appear to be large.

Based on the observation from the half Normal plot, now the ANOVA model is

$$y_{ijkl} = \mu + \tau_i + \beta_j + \gamma_k + (\tau\beta)_{ij} + (\tau\gamma)_{ik} + \varepsilon_{ijkl} \tag{1}$$

- τ_i is the effect of the ith `Temperature` level, $i = 1, 2$.
- β_j is the effect of the jth `CH2OConc` level, $j = 1, 2$.
- γ_k is the effect of the kth `StirRate` level, $j = 1, 2$.
- $(\tau\beta)_{ij}$ is the interaction effect of the ith `Temperature` level and the jth `CH2OConc` level.
- $(\tau\gamma)_{ij}$ is the interaction effect of the ith `Temperature` level and the kth `StirRate` level.
- ε_{ijkl} is the random error, $l = 1, 2$, satisfying

$$\varepsilon_{ijkl} \overset{i.i.d.}{\sim} N(0, \sigma^2) \text{ where } \sigma^2 \text{ is the conatnt variance.}$$

Use `aov()` to fit the ANOVA model.

```r
fit7 <- aov(
  FiltrationRate ~ factor(Temperature) * (factor(CH2OConc) + factor(StirRate)),
  data = df7
)
summary(fit7)
```

```
##                                       Df Sum Sq Mean Sq F value   Pr(>F)
## factor(Temperature)                    1 1870.6  1870.6   95.86 1.93e-06 ***
## factor(CH2OConc)                       1  390.1   390.1   19.99   0.0012 **
## factor(StirRate)                       1  855.6   855.6   43.85 5.92e-05 ***
```

```
## factor(Temperature):factor(CH2OConc)  1 1314.1  1314.1   67.34 9.41e-06 ***
## factor(Temperature):factor(StirRate)  1 1105.6  1105.6   56.66 2.00e-05 ***
## Residuals                            10  195.1    19.5
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Here, we left the interpretation of the response surface model for practice.

Addition of Center Points to a 2^k Designs

Recall the Resin Plant Experiment. Read the csv file `6_PilotPlant.csv` in R.

```r
df7 <- read.csv(file.path("data", "6_PilotPlant.csv"))
```

```r
df7_C <- data.frame(
  Temperature = rep(0, 4),
  Pressure = rep(0, 4),
  CH2OConc = rep(0, 4),
  StirRate = rep(0, 4),
  FiltrationRate = c(73, 75, 66, 69)
)
```

The calculation of $SS_{Purequadratic}$ with degree of freedom 1.

```r
Yf_bar <- mean(df7$FiltrationRate)
Yc_bar <- mean(df7_C$FiltrationRate)
nf <- nrow(df7)
nc <- nrow(df7_C)
SS_pureQuad <- nf*nc*(Yf_bar - Yc_bar)^2/(nf + nc)
```

The calculation of SS_E with degree of freedom $n_c - 1$.

```r
SS_E <- sum((df7_C$FiltrationRate - mean(df7_C$FiltrationRate))^2)
```

To test the significance of the Curvature, we compute the ratio of $MS_{Purequadratic}$ and MS_E as the F-statistic which follows the F distribution with degrees of freedom 1 and $n_c - 1$.

```r
MS_pureQuad <- SS_pureQuad/1
MS_E <- SS_E/(nc - 1)
fval <- MS_pureQuad/MS_E
pval <- 1 - pf(fval, 1, nc - 1) # p-value
```

The part of the testing the significance of the Curvature of the ANOVA table.

```r
print(data.frame(
  Source = c("Curvature", "Residual"),
  SS = c(SS_pureQuad, SS_E),
  DF = c(1, nc - 1),
  MS = c(MS_pureQuad, MS_E),
  "F" = c(sprintf("%.3f", fval), ""),
  "Pr(>F)" = c(sprintf("%.3f", pval), "")
))
```

```
##      Source      SS DF      MS     F Pr..F.
## 1 Curvature  1.5125  1  1.5125 0.093  0.780
## 2  Residual 48.7500  3 16.2500
```