01NAEX - Lecture 06
2^k Factorial Design

Exploring Experimental Designs for Multiple Factors

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2^k Factorial Design

Last lesson: Introduction to 2^k Factorial Design

- 2^k factorial design is widely used in industrial experimentation, especially in the early stages of experimental work, when many factors are likely to be investigated.
- Special case of the general factorial design with k factors, all at 2 levels, usually called low (-) and high (+).
- Factors are fixed, the design is completely randomized, and the usual normality assumptions are satisfied.

Today's lesson:

- pyDOE3 in Python, FrF2 package in R.
- Daniel Plot: Normal and Half-Normal Plot Effects.
- Pareto plot: Lenth's method.

General 2^k Factorials (Overview & Notation)

Design: k two-level factors $\Rightarrow N = 2^k$ runs.

Levels coding: $-1, +1$.

Regression Model (no replication):

$$y = \beta_0 + \sum_i \beta_i x_i + \sum_{i<j} \beta_{ij} x_i x_j + \cdots + \beta_{12\cdots k} x_1 \cdots x_k + \varepsilon.$$

General 2^k Factorial Design has

- k main effects
- $\binom{k}{2}$ two-factor interactions (first order interaction effects)
- $\binom{k}{3}$ three-factor interactions (second order interaction effects)
- $\vdots$
- 1 k-factor interaction

2^k Factorial Design - (Overview & Notation)

Effect estimates (orthogonal coding):

- Contrast for effect E: $C_E = \sum_{\text{runs}} s_r\, y_r$, where $s_r \in \{-1, +1\}$ is the column for E.
- Estimated effect: $\hat{E} = C_E / 2^{k-1}$.
- Sum of Squares: $\mathrm{SS}_E = C_E^2 / 2^k$.

Unreplicated (single replicated) 2^k Factorial Design:

- If the factors are spaced too closely, it increases the chances that the noise will overwhelm the signal in the data.
- More aggressive spacing is usually best.
- Lack of replication causes potential problems in statistical testing.
- With no replication:
  - Fitting the full model results in zero degrees of freedom for error.
  - Pooling tiny effects (high-order interactions) to estimate error.
  - σ^2 can be estimated by Daniel/half-normal/Lenth.

2^3 Factorial Design in R - FrF2 package (Plasma Etch Rate Experiment)

Back to Plasma Etch Rate Experiment from the last lesson - R

```
> FrF2(2^3, 3, replications = 2, randomize = FALSE,
               factor.names = c("Gap", "Flow", "Power"))
creating full factorial with  8  runs ...
run.no run.no.std.rp         Gap Flow  Power
 1          1.1               -1   -1    -1
 2          2.1                1   -1    -1
 3          3.1               -1    1    -1
 4          4.1                1    1    -1
 5          5.1               -1   -1     1
 6          6.1                1   -1     1
 7          7.1               -1    1     1
 8          8.1                1    1     1
 9          1.2               -1   -1    -1
10          2.2                1   -1    -1
11          3.2               -1    1    -1
12          4.2                1    1    -1
13          5.2               -1   -1     1
14          6.2                1   -1     1
15          7.2               -1    1     1
16          8.2                1    1     1
class=design, type= full factorial
```

2^3 Factorial Design in R - FrF2 package (Plasma Etch Rate Experiment)

Care about settings: `randomize = TRUE` or `randomize = FALSE`

```
> FrF2(2^3, 3, replications = 2, randomize = T,
              factor.names = c("Gap", "Flow", "Power"))
creating full factorial with  8  runs ...
run.no  run.no.std.rp    Gap Flow  Power
 1          7.1          -1    1     1
 2          6.1           1   -1     1
 3          3.1          -1    1    -1
 4          5.1          -1   -1     1
 5          4.1           1    1    -1
 6          8.1           1    1     1
 7          2.1           1   -1    -1
 8          1.1          -1   -1    -1
 9          3.2          -1    1    -1
10          2.2           1   -1    -1
11          6.2           1   -1     1
12          5.2          -1   -1     1
13          8.2           1    1     1
14          7.2          -1    1     1
15          4.2           1    1    -1
16          1.2          -1   -1    -1
class=design, type= full factorial
```

2^k Factorial Design in R - FrF2 package

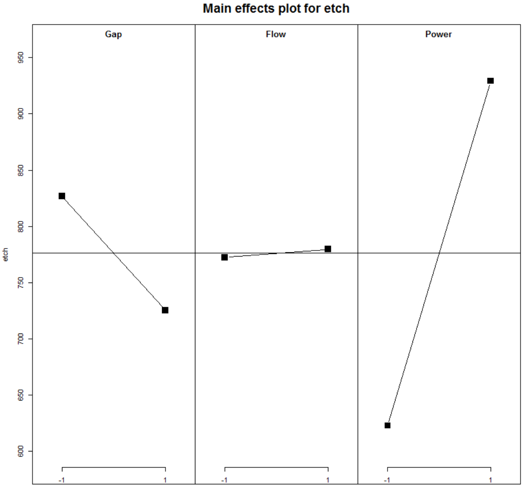
Back to Plasma Etch Rate Experiment - R

```
k = 3
plan <-  FrF2(2^k, k, replications = 2, randomize = FALSE,
factor.names = c("Gap", "Flow", "Power"))
plan <- add.response(plan, etch)
> plan
Gap Flow Power etch        Gap Flow Power etch
1   -1   -1    -1  550      9   -1   -1    -1  604
2    1   -1    -1  669      10   1   -1    -1  650
3   -1    1    -1  633      11  -1    1    -1  601
4    1    1    -1  642      12   1    1    -1  635
5   -1   -1     1 1037      13  -1   -1     1 1052
6    1   -1     1  749      14   1   -1     1  868
7   -1    1     1 1075      15  -1    1     1 1063
8    1    1     1  729      16   1    1     1  860
```

Analysis - same as in the last lesson.

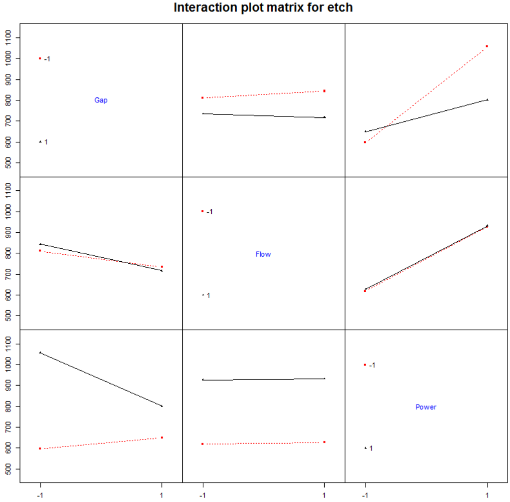
2^k Factorial Design in R - FrF2 package

```
MEPlot(plan)
```



2^k Factorial Design in R - FrF2 package

```
IAPlot(plan)
```



Unreplicated 2^k Factorial Designs

The 2^4 factorial design was used to investigate the effects of four factors on the filtration rate of a resin for a chemical process plant. The factors are:

A: temperature,

B: pressure,

C: concentration of chemical formaldehyde,

D: stirring rate.

Run Number	Factor *A*	*B*	*C*	*D*	Run Label	Filtration Rate (gal/h)
1	−	−	−	−	(1)	45
2	+	−	−	−	*a*	71
3	−	+	−	−	*b*	48
4	+	+	−	−	*ab*	65
5	−	−	+	−	*c*	68
6	+	−	+	−	*ac*	60
7	−	+	+	−	*bc*	80
8	+	+	+	−	*abc*	65
9	−	−	−	+	*d*	43
10	+	−	−	+	*ad*	100
11	−	+	−	+	*bd*	45
12	+	+	−	+	*abd*	104
13	−	−	+	+	*cd*	75
14	+	−	+	+	*acd*	86
15	−	+	+	+	*bcd*	70
16	+	+	+	+	*abcd*	96

$2^4 = 16$ runs were made in random order.

Unreplicated 2^k Factorial Designs

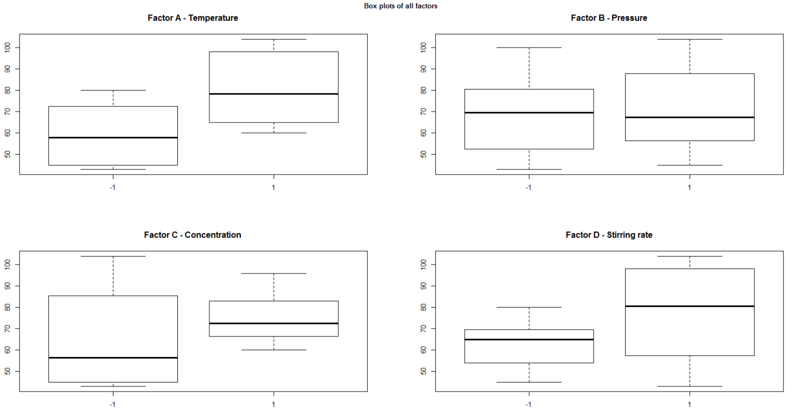
Pilot Plant Filtration Rate Experiment - FrF2 package

```
> rate=FrF2(2^4, 4, replications = 1,
       randomize = FALSE,factor.names = c("A", "B", "C", "D"
> Filtration = rate_experiment$Rate
> rate       = add.response(rate, Filtration)
> summary(rate)
Experimental design of type  full factorial 16  runs

Factor settings:      Responses:
A  B  C  D           [1] Filtration
1 -1 -1 -1 -1
2  1  1  1  1
The design itself:
   A  B  C  D Filtration    A  B  C  D Filtration
1  -1 -1 -1 -1         45   -1 -1 -1  1         43
2   1 -1 -1 -1         71    1 -1 -1  1        100
3  -1  1 -1 -1         48   -1  1 -1  1         45
4   1  1 -1 -1         65    1  1 -1  1        104
5  -1 -1  1 -1         68   -1 -1  1  1         75
6   1 -1  1 -1         60    1 -1  1  1         86
7  -1  1  1 -1         80   -1  1  1  1         70
8   1  1  1 -1         65    1  1  1  1         96
```

Pilot Plant Filtration Rate Experiment

Box plot

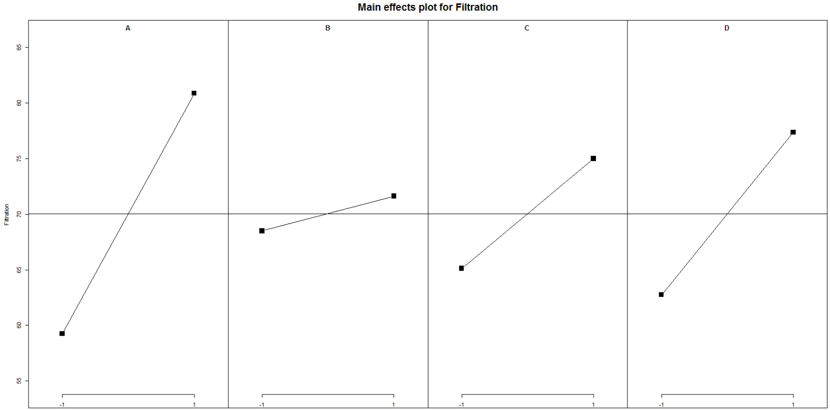
```
boxplot(Filtration ~ A , main = "Factor A - Temperature")
```



Pilot Plant Filtration Rate Experiment

Main Effects plotfor response variable

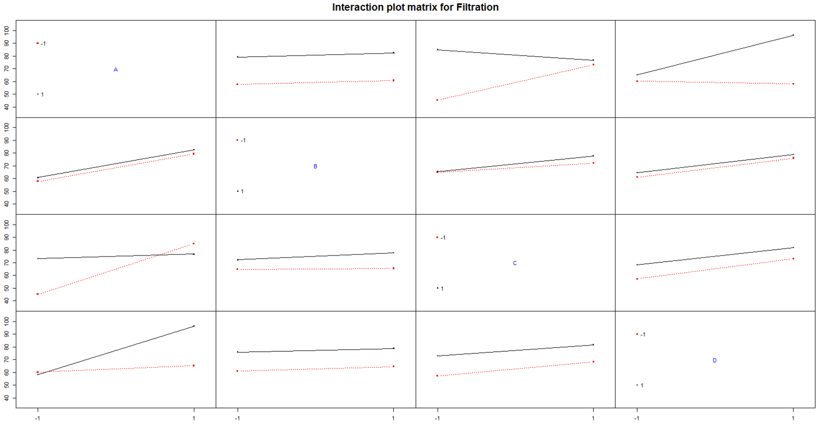
```
MEPlot(plan)
```



Pilot Plant Filtration Rate Experiment

Interaction Plot matrix for response variable

```
IAPlot(plan)
```



Pilot Plant Filtration Rate Experimene

ANOVA table - model with all factors and interactions

```
anova(aov(Filtration~A*B*C*D,  data=rate))
  Analysis of Variance Table, Response: Filtration
               Df  Sum Sq Mean Sq F value Pr(>F)
  A             1 1870.56 1870.56
  B             1   39.06   39.06
  C             1  390.06  390.06
  D             1  855.56  855.56
  A:B           1    0.06    0.06
  A:C           1 1314.06 1314.06
  B:C           1   22.56   22.56
  A:D           1 1105.56 1105.56
  B:D           1    0.56    0.56
  C:D           1    5.06    5.06
  A:B:C         1   14.06   14.06
  A:B:D         1   68.06   68.06
  A:C:D         1   10.56   10.56
  B:C:D         1   27.56   27.56
  A:B:C:D       1    7.56    7.56
  Residuals     0    0.00
  Warning message: ANOVA F-tests are unreliable
```

Pilot Plant Filtration Rate Experimene: LM - all factors and interactions

```
> summary(lm(Filtration~A*B*C*D,  data=rate))
ALL 16 residuals are 0: no residual degrees of freedom!
             Estimate    Std. Error t value Pr(>|t|)
(Intercept)  70.0625          NA       NA        NA
A1           10.8125          NA       NA        NA
B1            1.5625          NA       NA        NA
C1            4.9375          NA       NA        NA
D1            7.3125          NA       NA        NA
A1:B1         0.0625          NA       NA        NA
A1:C1        -9.0625          NA       NA        NA
B1:C1         1.1875          NA       NA        NA
A1:D1         8.3125          NA       NA        NA
B1:D1        -0.1875          NA       NA        NA
C1:D1        -0.5625          NA       NA        NA
A1:B1:C1      0.9375          NA       NA        NA
A1:B1:D1      2.0625          NA       NA        NA
A1:C1:D1     -0.8125          NA       NA        NA
B1:C1:D1     -1.3125          NA       NA        NA
A1:B1:C1:D1   0.6875          NA       NA        NA
Residual standard error: NaN on 0 degrees of freedom
Multiple R-squared: 1, Adjusted R-squared: NaN
F-statistic: NaN on 15 and 0 DF, p-value: NA
```

Pilot Plant Filtration Rate Experimene

ANOVA table - model with all factors and interactions in Python

```
import statsmodels.api as sm
from statsmodels.formula.api import ols

# Define the model
model=ols('EtchRate ~ Gap*Flow*Power', data=design_df).fit()

# Perform ANOVA
anova_table = sm.stats.anova_lm(model, typ=2)
print(anova_table)
```

Analysis of significant effects

We can't use usual way because:

- ANOVA gives SS but no error estimate!
- LM gives effect estimates but no error estimate!
- We try to adjust a 2^k dimensional model to 2^k observations, leaving 0 dimensions (degrees of freedom) for the error estimate.

We don't know σ and we can't estimate it. We know that

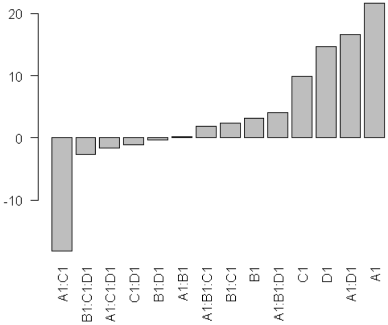
- the effects estimates are normally distributed with mean 0 and common standard deviation σ.
- the effect estimates are independent.

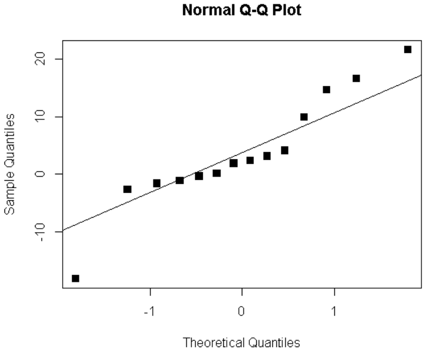
Lets make *QQ*-plot and look for the outliers - suspected significant effects.

Analysis of significant effects

Make QQ plot from Linear Model coefficients (without intercept) manually:

```
> model0 = lm(2*Filtration~A*B*C*D,  data=rate)
> barplot(sort(model0$coeff[2:(2^4-1)]),las = 2)
> qqnorm(model0$coeff[2:(2^4-1)],cex = 1.3,pch = 15)
> qqline(model0$coeff[2:(2^4-1)],cex = 1.3,pch = 15)
```





Daniel plot

Daniel plot is the normal probability plot of the estimated effects.

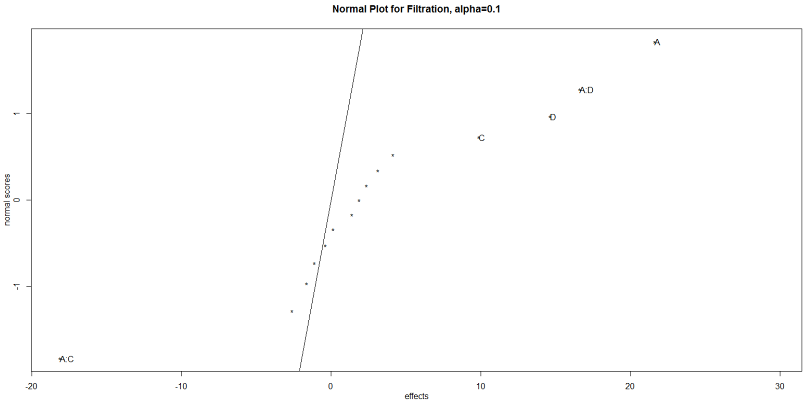
The effects that are negligible are normally distributed, with mean zero and variance σ^2 and will tend to fall along a straight line on this plot, whereas significant effects will have nonzero means and will not lie along straight line.

1. **Negligible effects**: lie along the qqline.
2. **Important effects**: lie far from the qqline.

Pilot Plant Filtration Rate Experiment

Daniel Plot (Classical effects qqplot) with alpha = 0.1, qqline, and only significant factors

```
qqplot(DanielPlot(rate,alpha=0.1)$x,DanielPlot(rate)$y)
qqline(DanielPlot(rate,alpha=0.1)$y)
```



The Half-Normal Plot Effects

Alternative plot to the Normal probability plot:

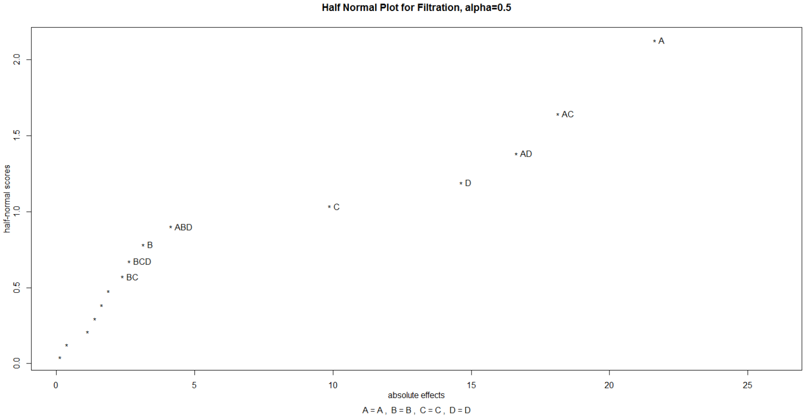
It is a plot of absolute value of the effects estimates against their cumulative normal probabilities.

The straight line on the half-normal plot always passes through the origin and should pass close to the fiftieth percentile data value. Bettet for interpretation with a few effects estimates (for example 8-run design).

Pilot Plant Filtration Rate Experimene

Half normal plot of effects

```
DanielPlot(rate,code=TRUE,alpha=0.1,half=TRUE)
```



Lenth's method - Pareto plot

Method proposed by Lenth (1989), sometime called Pareto plot has good power to detect significant effects.

Suppose we have m contrast of interest $c_1, c_2, \ldots c_m$. For 2^k unreplicated factor design $m = 2^k - 1$. Lenth's method estimates the variance of a contrast from the smallest contrast estimate.

$$s_0 = 1.5\text{median}(|c_j|) \quad PSE = 1.5\text{median}(|c_j|\,,\ |c_j| < 2.5 s_0)$$

PSE is called pseudostandard error and it should be reasonable estimator of the contrast variance. An individual contrast is compared to the **margin of error**:

$$ME = t_{0.025,d} PSE, \quad d = \frac{m}{3}$$

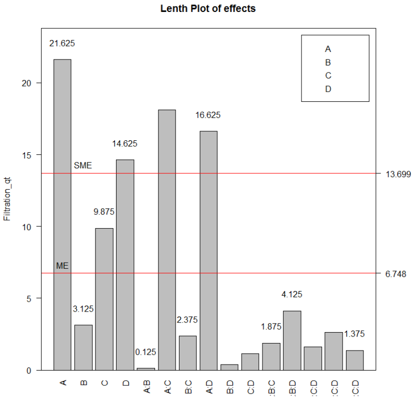
or to the **simultaneous margin of error**

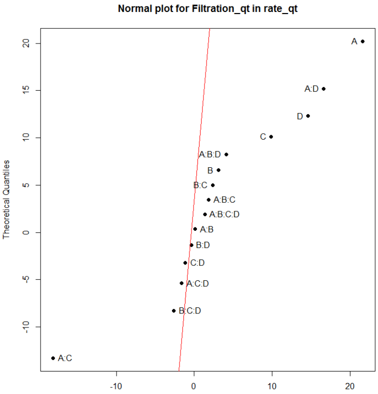
$$SME = t_{\gamma,d} PSE, \quad \gamma = 1 - \frac{(1 + 0.95^{\frac{1}{m}})}{2}$$

Pilot Plant Filtration Rate Experimene - qualityTools library

```
rate_pareto = fracDesign(k = 4, replicates = 1)
response(rate_pareto) = rate$Filtration[rate_pareto[,1]]
paretoPlot(rate_pareto) normalPlot(rate_pareto)
```

$PSE = 1.5 \times |1.75| = 2.625$, $ME = 2.571 \times 2.625 = 6.748$, $SME = 5.219 \times 2.625 = 13.699$





Daniel vs Half-Normal vs Lenth (Summary When No Replication)

Daniel (normal QQ): plot effect estimates $\hat{E}$ vs normal quantiles. Active effects depart from the line.

Half-normal: plot $|\hat{E}|$ vs half-normal quantiles; no sign ambiguity.

Lenth PSE & Pareto: robust pseudo-σ from small effects,

$$s_0 = 1.5\,\mathrm{median}(|c_j|),\; PSE = 1.5\,\mathrm{median}\{|c_j| : |c_j| < 2.5 s_0\},$$

then thresholds via

$$ME = t_{0.025,d}\,PSE,\; d = m/3.$$

Build a Pareto of $|c_j|$ with ME/SME lines.

Pilot Plant Filtration Rate Experimene

ANOVA table - model without factor B

By having dropped B totally, we obtain a 2^3 design with 2 replicates per cell.

```
> anova(aov(Filtration~A*C*D,  data=rate))
Analysis of Variance Table

Response: Filtration
Df   Sum Sq Mean Sq F value    Pr(>F)
A          1 1870.56 1870.56 83.3677 1.667e-05 ***
C          1  390.06  390.06 17.3844 0.0031244 **
D          1  855.56  855.56 38.1309 0.0002666 ***
A:C        1 1314.06 1314.06 58.5655 6.001e-05 ***
A:D        1 1105.56 1105.56 49.2730 0.0001105 ***
C:D        1    5.06    5.06  0.2256 0.6474830
A:C:D      1   10.56   10.56  0.4708 0.5120321
Residuals  8  179.50   22.44
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1  1
>
```

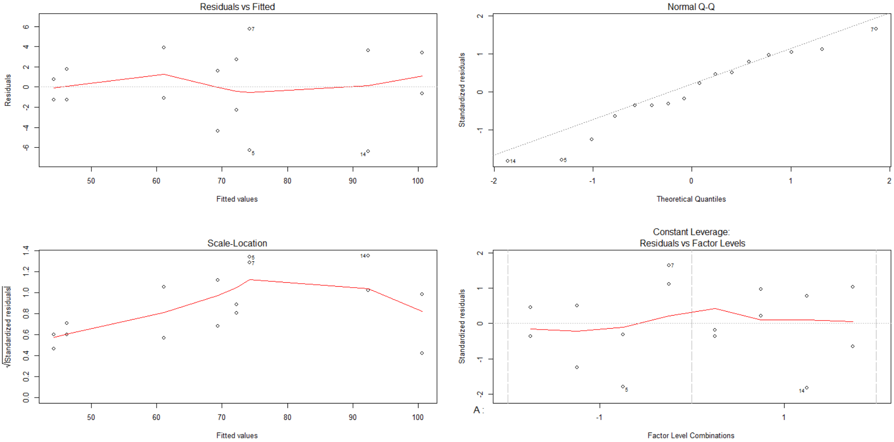
Pilot Plant Filtration Rate Experimene

ANOVA table - final model

```
> anova(aov(Filtration~A*C+A*D,  data=rate))
Analysis of Variance Table

Response: Filtration
Df   Sum Sq Mean Sq F value    Pr(>F)
A          1 1870.56 1870.56  95.865 1.928e-06 ***
C          1  390.06  390.06  19.990  0.001195 **
D          1  855.56  855.56  43.847 5.915e-05 ***
A:C        1 1314.06 1314.06  67.345 9.414e-06 ***
A:D        1 1105.56 1105.56  56.659 1.999e-05 ***
Residuals 10  195.12   19.51
--
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
>
```

Pilot Plant Filtration Rate Experiment

Model validation



+ perform all relevant statistical hypothesis testing.

Pilot Plant Filtration Rate Experimene

Another approach - omitting the highest interaction

```
>anova(aov(Filtration~(.)^3,  data=rate))
Analysis of Variance Table, Response: Filtration
Df   Sum Sq Mean Sq  F value  Pr(>F)
A           1 1870.56 1870.56 247.3471 0.04042 *
B           1   39.06   39.06   5.1653 0.26388
C           1  390.06  390.06  51.5785 0.08808 .
D           1  855.56  855.56 113.1322 0.05968 .
A:B         1    0.06    0.06   0.0083 0.94228
A:C         1 1314.06 1314.06 173.7603 0.04820 *
A:D         1 1105.56 1105.56 146.1901 0.05253 .
B:C         1   22.56   22.56   2.9835 0.33410
B:D         1    0.56    0.56   0.0744 0.83050
C:D         1    5.06    5.06   0.6694 0.56345
A:B:C       1   14.06   14.06   1.8595 0.40282
A:B:D       1   68.06   68.06   9.0000 0.20483
A:C:D       1   10.56   10.56   1.3967 0.44707
B:C:D       1   27.56   27.56   3.6446 0.30718
Residuals   1    7.56    7.56
```

Continue only with significant variables.

Pilot Plant Filtration Rate Experiment - Regression analysis

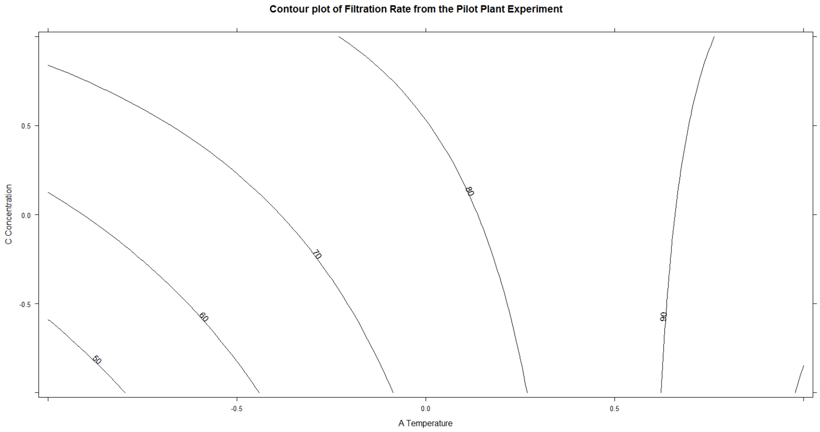
Preparation for countour plots (Swap factors for numerics)

```
> rate$A.num <- 2*(as.numeric(rate$A)-1.5)
> rate$C.num <- 2*(as.numeric(rate$C)-1.5)
> rate$D.num <- 2*(as.numeric(rate$D)-1.5)
> rate.lm       <- lm(Filtration~A.num*C.num+A.num*D.num,data=rate)
> summary(rate.lm)

Coefficients: Estimate Std. Error t value Pr(>|t|)
(Intercept)   70.062      1.104   63.444 2.30e-14 ***
A.num         10.812      1.104    9.791 1.93e-06 ***
C.num          4.938      1.104    4.471   0.0012 **
D.num          7.313      1.104    6.622 5.92e-05 ***
A.num:C.num   -9.063      1.104   -8.206 9.41e-06 ***
A.num:D.num    8.312      1.104    7.527 2.00e-05 ***
Residual standard error: 4.417 on 10 degrees of freedom
Multiple R-squared: 0.966,  Adjusted R-squared: 0.9489
F-statistic: 56.74 on 5 and 10 DF,  p-value: 5.14e-07

> tmp          <- list(A.num=seq(-1,1,by=.05),C.num=seq(-1,1,by=0.05
D.num=seq(-1,1,by=0.05),data=rate)
> new.data     <- expand.grid(tmp)
> new.data$fit<- predict(rate.lm,new.data)
```

Pilot Plant Filtration Rate Experiment

Countour plot: A(temperature) and C(concentration) interaction only

```
contourplot(fit~A.num*C.num,new.data,xlab="A Temperature",
ylab="C Concentration",
main="Contour plot of Filtration Rate from the Pilot Plant Experime
```

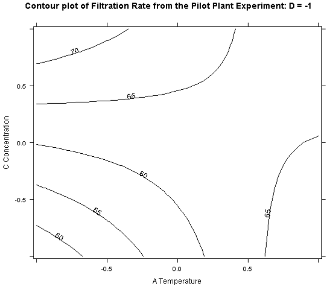


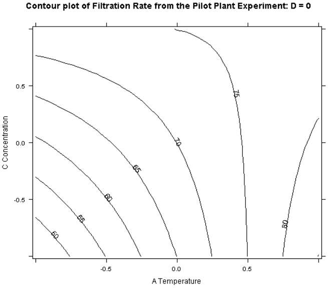
No specification in the code means last value of D, i.e. D = 1.

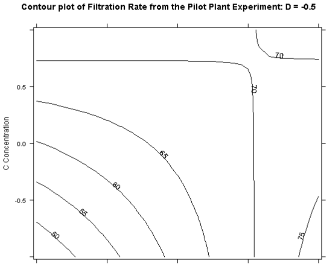
Pilot Plant Filtration Rate Experiment

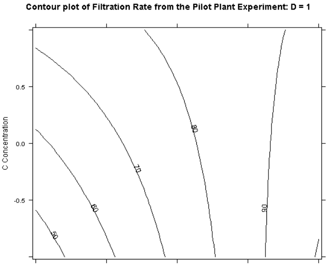
Countour plot: A(temperature) and C(concentration) for different D's.

```
contourplot(fit~A.num*C.num,new.data[new.data$D.num == -1,])
```





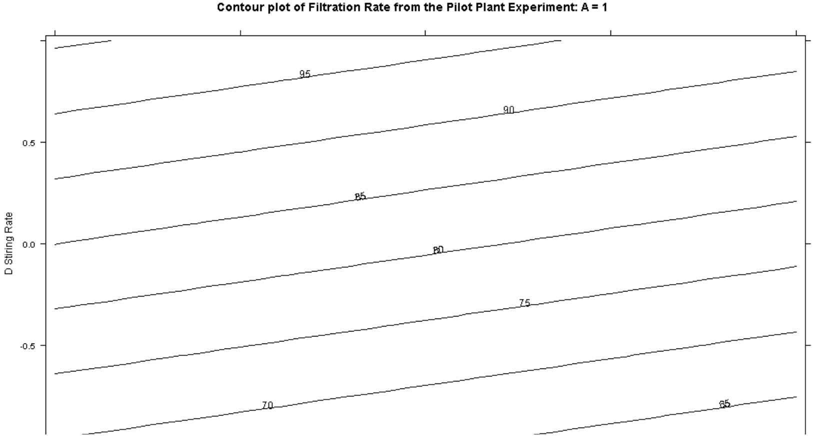




Pilot Plant Filtration Rate Experiment

Countour plot: C(concentration) and D(stirring rate) interaction only

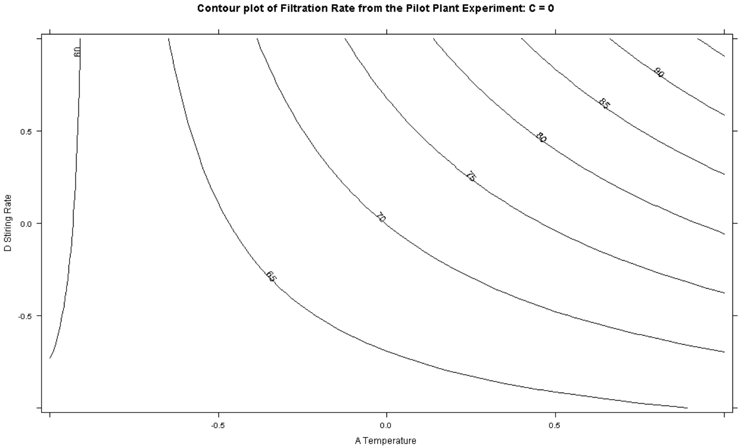
```
> contourplot(fit~C.num*D.num,new.data[new.data$A.num == 1,],
 xlab="C Concentration",ylab="D Stiring Rate",
 main = "Contour plot of Filtration Rate from the Pilot Plant Exper
 A = 1")
```



Pilot Plant Filtration Rate Experiment

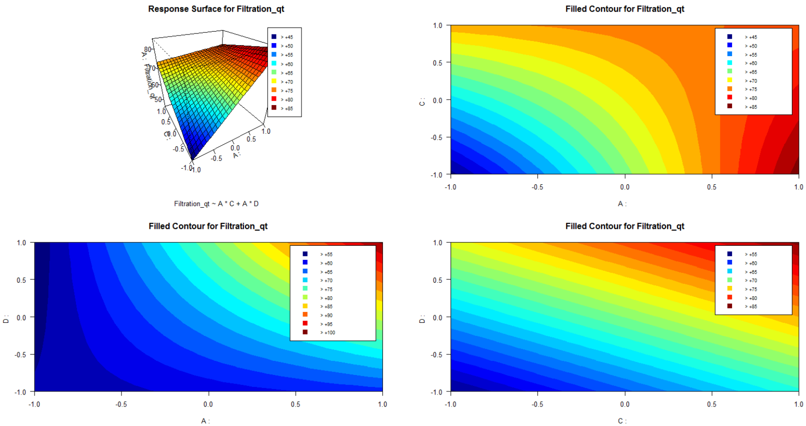
Countour plot: A(temperature) and D(stirring rate) interaction only

```
contourplot(fit~A.num*D.num,new.data[new.data$C.num == 0,],
xlab="A Temperature",ylab="D Stiring Rate",
main="Contour plot of Filtration Rate from the Pilot Plant Experiment
:C = 0")
```



Pilot Plant Filtration Rate Experiment

```
wirePlot(A, C, Filtration_qt, data = rate_qt)
contourPlot(A, C, Filtration_qt, data = rate_qt)
```



Missing factor is equal to 0 in all three cases!

Today Exercise

Solve problems 6.28 + 6.29 and 6.31 + 6.32 from the chapter 6,
D. C. Montgomery DAoE - 8. edition.
Don’t use center points and curvature terms
(will be covered in the next lesson).

Today Exercise

■ **TABLE P6.8**

The 2^4 Experiment for Problem 6.31

Run Number	Actual Run Order	A	B	C	D	Molecular Weight	Viscosity
1	18	−	−	−	−	2400	1400
2	9	+	−	−	−	2410	1500
3	13	−	+	−	−	2315	1520
4	8	+	+	−	−	2510	1630
5	3	−	−	+	−	2615	1380
6	11	+	−	+	−	2625	1525
7	14	−	+	+	−	2400	1500
8	17	+	+	+	−	2750	1620
9	6	−	−	−	+	2400	1400
10	7	+	−	−	+	2390	1525
11	2	−	+	−	+	2300	1500
12	10	+	+	−	+	2520	1500
13	4	−	−	+	+	2625	1420
14	19	+	−	+	+	2630	1490
15	15	−	+	+	+	2500	1500
16	20	+	+	+	+	2710	1600
17	1	0	0	0	0	2515	1500
18	5	0	0	0	0	2500	1460
19	16	0	0	0	0	2400	1525
20	12	0	0	0	0	2475	1500

Factor Levels	Low (−)	High (+)
A (°C)	100	120
B (%)	4	8
C (min)	20	30
D (psi)	60	75