STA305/1004-Class 24

March 30, 2016

Today's Class

- Assessing significance in unreplicated factorial designs
  - Normal plots
  - half-Normal plots
  - Lenth's method
- Blocking factorial designs
  - Effect hierarchy principle
  - Generation of orthogonal blocks
  - Generators and deining relations
- Fractional factorial design

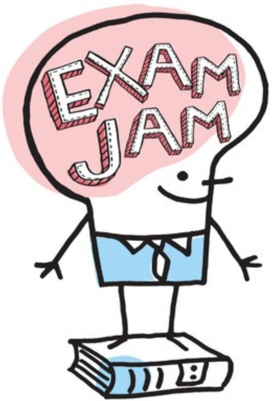
Exam review session

Date: Monday, April 11th

Time: 11 am - 12 noon

Location: SS 2102

Stop
by the SS lobby to take a few photos
in the Photobooth, enjoy some free
coffee and snacks and engage in other
fun activities (lobby activities run 11-3).



Example - 2^3 design for studying a chemical reaction

A process development experiment studied four factors in a 2^4 factorial design.

- amount of catalyst charge **1**,
- temperature **2**,
- pressure **3**,
- concentration of one of the reactants **4**.
- The response y is the percent conversion at each of the 16 run conditions. The design is shown below.

Example - 2^4 design for studying a chemical reaction

x1	x2	x3	x4	conversion
-1	-1	-1	-1	70
1	-1	-1	-1	60
-1	1	-1	-1	89
1	1	-1	-1	81
-1	-1	1	-1	69
1	-1	1	-1	62
-1	1	1	-1	88
1	1	1	-1	81
-1	-1	-1	1	60
1	-1	-1	1	49
-1	1	-1	1	88
1	1	-1	1	82
-1	-1	1	1	60
1	-1	1	1	52
-1	1	1	1	86
1	1	1	1	79

The design is not replicated so it's not possible to estimate the standard errors of the factorial effects.

Example - 2^4 design for studying a chemical reaction

factorial effects
$|||$
Regression slopes $\times 2$

```
fact1 <- lm(conversion~x1*x2*x3*x4,data=tab0510a)
round(2*fact1$coefficients,2)
```

```
(Intercept)          x1          x2          x3          x4       x1:x2
     144.50       -8.00       24.00       -0.25       -5.50        1.00
      x1:x3       x2:x3       x1:x4       x2:x4       x3:x4    x1:x2:x3
       0.75       -1.25        0.00        4.50       -0.25       -0.75
   x1:x2:x4    x1:x3:x4    x2:x3:x4 x1:x2:x3:x4
       0.50       -0.25       -0.75       -0.25
```

for fact. effects $\neq 0$
are they important?

Half-Normal Plots

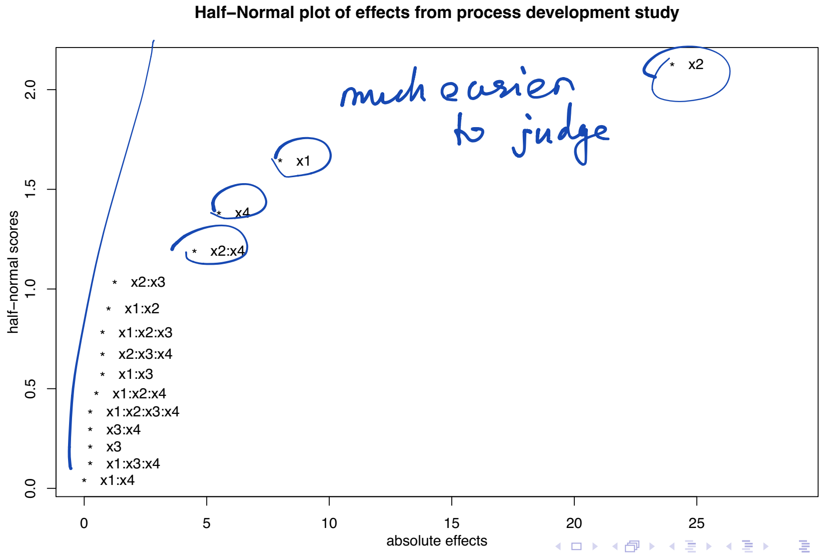
- A related graphical method is called the half-normal probability plot.
- Let
$$\left|\hat{\theta}\right|_{(1)} < \left|\hat{\theta}\right|_{(2)} < \cdots < \left|\hat{\theta}\right|_{(N)}.$$
denote the ordered values of the unsigned factorial effect estimates.
- Plot them against the coordinates based on the half-normal distribution - the absolute value of a normal random variable has a half-normal distribution.
- The half-normal probability plot consists of the points
$$\left|\hat{\theta}\right|_{(i)} \text{ vs. } \Phi^{-1}(0.5 + 0.5[i - 0.5]/N).\ i = 1, \ldots, N.$$

Half-Normal Plots

- An advantage of this plot is that all the large estimated effects appear in the upper right hand corner and fall above the line.
- The half-normal plot for the effects in the process development example is can be obtained with `DanielPlot()` with the option `half=TRUE`.

Half-Normal Plots

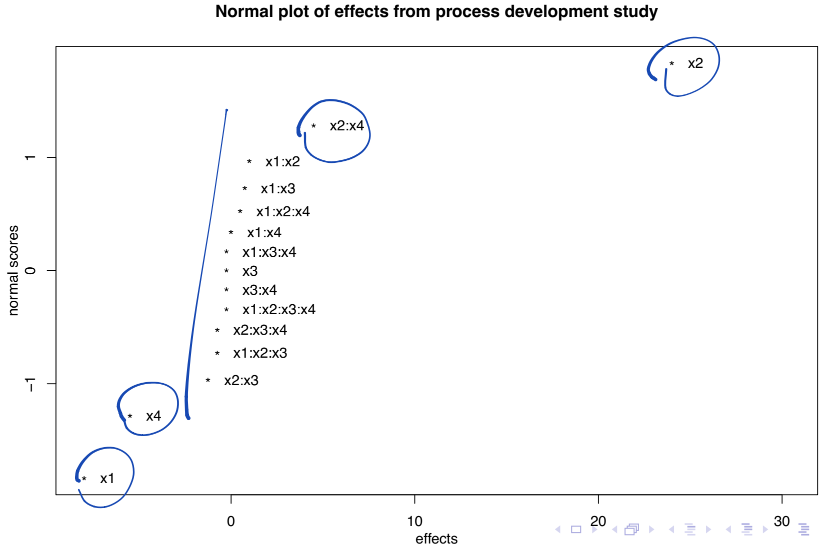
```
library(FrF2)
DanielPlot(fact1,half=TRUE,autolab=F,
        main="Half-Normal plot of effects from process development study")
```



Half-Normal Plots

Compare with full Normal plot.

```r
library(FrF2)
DanielPlot(fact1,half=F,autolab=F,
        main="Normal plot of effects from process development study")
```



Lenth's method

Russ Lenth

- Let

$$\hat{\theta}_{(1)}, \ldots, \hat{\theta}_{(N)}$$

be estimated factorial effects of $\theta_1, \theta_2, \ldots, \theta_N$ in a 2^k design $N = 2^k - 1$.

- Assume that all the factorial effects have the same standard deviation.
- The pseudo standard error (PSE) is defined as

$$PSE = 1.5 \cdot \text{median}_{|\hat{\theta}_i| < 2.5 s_0} \left|\hat{\theta}_i\right|,$$

- The median is computed among the $\left|\hat{\theta}_i\right|$ with $\left|\hat{\theta}_i\right| < 2.5 s_0$ and

$$s_0 = 1.5 \cdot \text{median} \left|\hat{\theta}_i\right|.$$

derived via a combination of
simulation & theory

Lenth's method

- $1.5 \cdot s_0$ is a consistent estimator of the standard deviation of $\hat{\theta}$ when $\theta_i = 0$ and the underlying distribution is normal.
- The $P(|Z| > 2.57) = 0.01, Z \sim N(0, 1)$.
- $\left|\hat{\theta}_i\right| < 2.5 s_0$ trims approximately 1% of the $\hat{\theta}_i$ if $\theta_i = 0$. why 2.5?
- The trimming attempts to remove the $\hat{\theta}_i$ associated with non-zero (active) effects.
- By using the median in combination with the trimming means that *PSE* is not sensitive to the $\hat{\theta}_i$ associated with active effects.

Lenth's method

if $\hat{\theta} < ME$ then not sig. (interval contains 0)

$\hat{\theta} \pm ME$

- To obtain a margin of error Lenth suggested multiplying the PSE by the $100 * (1 - \alpha)$ quantile of the t_d distribution, $t_{d,\alpha/2}$.
- The degrees of freedom is $d = N/3$. For example, the margin of error for a 95% confidence interval for θ_i is

$$ME = t_{d,.025} \times PSE.$$

- All estimates greater than the ME may be viewed as "significant", but with so many estimates being considered simultaneously, some will be falsely identified.
- A simultaneous margin of error that accounts for multiple testing can also be calculated,

e.g. - 2^3

1, 2, 3, 12, 13, 23, 123

$$SME = t_{d,\gamma} \times PSE,$$

where $\gamma = \left(1 + 0.95^{1/N}\right)/2$.

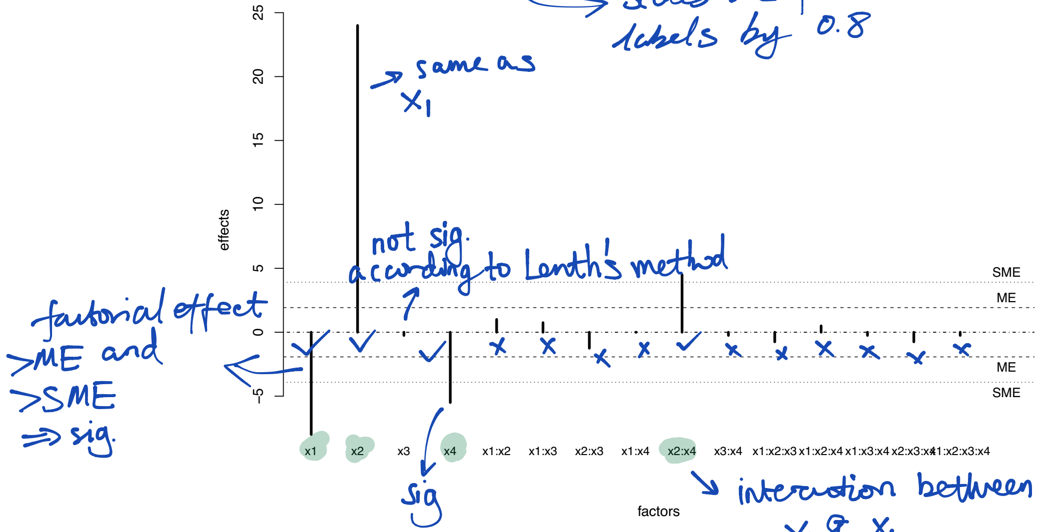
7 factorial designs

- The details of how to calculate MSE and PSE are given in the class notes.

Lenth's method - Lenth Plot for process development example

```r
LenthPlot(fact1,cex.fac = 0.8)
```

scales the factor labels by 0.8




```
##     alpha      PSE       ME      SME
## 0.050000 0.750000 1.927936 3.913988
```

Blocking factorial designs

- In a trial conducted using a 2^3 design it might be desirable to use the same batch of raw material to make all 8 runs.
- Suppose that batches of raw material were only large enough to make 4 runs. Then the concept of blocking could be used.

Blocking factorial designs

Consider the 2^3 design.

Run	1	2	3	12	13	23	123
1	-1	-1	-1	1	1	1	-1
2	1	-1	-1	-1	-1	1	1
3	-1	1	-1	-1	1	-1	1
4	1	1	-1	1	-1	-1	-1
5	-1	-1	1	1	-1	-1	1
6	1	-1	1	-1	1	-1	-1
7	-1	1	1	-1	-1	1	-1
8	1	1	1	1	1	1	1

go to block I

go to block II

Sign 123

Runs	Block
1, 4, 6, 7	I
2, 3, 5, 8	II

-1

+1

How are the runs assigned to the blocks?

Blocking factorial designs

Run	1	2	3	12	13	23	123
1	-1	-1	-1	1	1	1	-1
2	1	-1	-1	-1	-1	1	1
3	-1	1	-1	-1	1	-1	1
4	1	1	-1	1	-1	-1	-1
5	-1	-1	1	1	-1	-1	1
6	1	-1	1	-1	1	-1	-1
7	-1	1	1	-1	-1	1	-1
8	1	1	1	1	1	1	1

Runs	Block	sign of 123
1, 4, 6, 7	I	$-$
2, 3, 5, 8	II	$+$

Blocking factorial designs

- Any systematic differences between the two blocks of four runs will be eliminated from all the main effects and two factor interactions.
- What you gain is the elimination of systematic differences between blocks.
- But now the three factor interaction is confounded with any batch (block) difference.
- The ability to estimate the three factor interaction separately from the block effect is lost.

Effect hierarchy principle

main-effect & 2-way interaction effects

1. Lower-order effects are more likely to be important than higher-order effects.
2. Effects of the same order are equally likely to be important.

- One reason that many accept this principle is that higher order interactions are more difficult to interpret or justify physically.
- Investigators are less interested in estimating the magnitudes of these effects even when they are statistically significant.

OK to give up higher order effects to use for blocks

Generation of Orthogonal Blocks

In the 2^3 example suppose that the block variable is given the identifying number 4.

Run	1	2	3	4=123
1	-1	-1	-1	-1
2	1	-1	-1	1
3	-1	1	-1	1
4	1	1	-1	-1
5	-1	-1	1	1
6	1	-1	1	-1
7	-1	1	1	-1
8	1	1	1	1

- Think of your experiment as containing four factors.
- The fourth factor will have the special property that it does not interact with other factors.
- If this new factor is introduced by having its levels coincide exactly with the plus and minus signs attributed to 123 then the blocking is said to be **generated** by the relationship 4=123.
- This idea can be used to derive more sophisticated blocking arrangements.

An example of how not to block

Suppose we would like to arrange the 2^3 design into four blocks.

Run	1	2	3	4=123	5=23	45=1
1	-1	-1	-1	-1	1	-1
2	1	-1	-1	1	1	1
3	-1	1	-1	1	-1	-1
4	1	1	-1	-1	-1	1
5	-1	-1	1	1	-1	-1
6	1	-1	1	-1	-1	1
7	-1	1	1	-1	1	-1
8	1	1	1	1	1	1

- Runs are placed in different blocks depending on the signs of the block variables in columns 4 and 5.
- Consider two block factors called 4 and 5.
- 4 is associated with ? 123 → 3-way interaction
- 5 is associated ? 23 → 2-way interaction

An example of how not to block

Blocking vars are 4 & 5

Run	1	2	3	4=123	5=23	45=1
1	-1	-1	-1	-1	1	-1
2	1	-1	-1	1	1	1
3	-1	1	-1	1	-1	-1
4	1	1	-1	-1	-1	1
5	-1	-1	1	1	-1	-1
6	1	-1	1	-1	-1	1
7	-1	1	1	-1	1	-1
8	1	1	1	1	1	1

main effect of 1 = interaction between 4.5

multiple 4,5 main effect ?

block this way = loss ability to est. main effect of 1.

4 batches raw material

how to assign runs to batches?

Block	Run
I	4, 6
II	3, 5
III	1, 7
IV	2, 8

sign of 4	5
−	−
+	−
−	+
+	+

An example of how not to block

- 45 is confounded with the main effect of 1.
- Therefore, if we use 4 and 5 as blocking variables we will not be able to estimate the main effect 1.
- Main effects should not be confounded with block effects.

(mixed up with)

An example of how not to block

according to effects of hierarchy principle

- Any blocking scheme that confounds main effects with blocks should not be used.
- This is based on the assumption:

  The block-by-treatment interactions are negligible.

- This assumption states that treatment effects do not vary from block to block.
- Without this assumption estimability of the factorial effects will be very complicated.

An example of how not to block

$1 \cdot 1 = I =$ column of $+1$'s

$2 \cdot 2 = I =$

- For example, if $B_1 = 12$ then this implies two other relations:

$$1B_1 = 112 = 2 \text{ and } B_1 2 = 122 = 122 = 1.$$

- If there is a significant interaction between the block effect B_1 and the main effect 1 then the main effect 2 is confounded with $1B_1$.
- If there is a significant interaction between the block effect B_1 and the main effect 2 then the main effect 1 is confounded with $B_1 2$.

How to do it

Run	1	2	3	4=12	5=13
1	-1	-1	-1	1	1
2	1	-1	-1	-1	-1
3	-1	1	-1	-1	1
4	1	1	-1	1	-1
5	-1	-1	1	1	-1
6	1	-1	1	-1	1
7	-1	1	1	-1	-1
8	1	1	1	1	1

I = column of +1

$4=12 \qquad 4\cdot 4 = I = 12\cdot 4$

$5=13 \Rightarrow 5\cdot 5 = I = 13\cdot 5$

$4\cdot 5 = 12\cdot 13 = 2\cdot 1\cdot 13 = 2\cdot I\cdot 3$

$= 23$

Block	4	5	run
I	−	−	2, 7
II	−	+	3, 6
III	+	−	4, 5
IV	+	+	1, 8

- Set 4=12, 5=13.
- Then $I = 124 = 135 = 2345$.
- Estimated block effects 4, 5, 45 are assoicated with the estimated two-factor interaction effects 12, 13, 23 and not any main effects.
- Which runs are assigned to which blocks?

Generators and Defining Relations

- A simple calculus is available to show the consequences of any proposed blocking arrangement.
- If any column in a 2^k design are multiplied by themselves a column of plus signs is obtained. This is denoted by the symbol I.

$$I = 11 = 22 = 33 = 44 = 55,$$

where, for example, 22 means the product of the elements of column 2 with itself.

- Any column multiplied by I leaves the elements unchanged. So, $I3 = 3$.

Generators and Defining Relations

- A general approach for arranging a 2^k design in 2^q blocks of size 2^{k-q} is as follows.
- Let $B_1, B_2, \ldots, B_q$ be the block variables and the factorial effect v_i is confounded with B_i,

$$B_1 = v_1, B_2 = v_2, \ldots, B_q = v_q.$$

- The block effects are obtained by multiplying the B_i's:

$$B_1 B_2 = v_1 v_2, B_1 B_3 = v_1 v_3, \ldots, B_1 B_2 \cdots B_q = v_1 v_2 \cdots v_q$$

- There are $2^q - 1$ possible products of the B_i's and the I (whose components are $+$).

Generators and Defining Relations

② $B_1 = 12, B_2 = 13, B_3 = 45$

$B_1 \cdot B_2 = 1213 = 23$

$B_1 \cdot B_3 = 1245$

$B_2 \cdot B_3 = 1345$

$B_1 B_2 B_3 = 121345 = 2345$

Second blocking scheme is associated with 12, 13, 45, 23, 1245, 1345, 2345

4 2-way

What do I look at?

① $B_1 = 135, B_2 = 235, B_3 = 1234$

$2^5 = 32$

Run	1	2	3	4	5	12	23
1	−	−					
2	+	−					
3	−	+					
⋮							

$B_1 \cdot B_2 = 135 \cdot 235 = 153 \cdot 325 = 15I25 = 1552 = 12$

$B_1 \cdot B_3 = 135 \cdot 1234 = 524$

$B_2 \cdot B_3 = 235 \cdot 1234 = 154$

$B_1 \cdot B_2 \cdot B_3 = 135 \cdot 235 \cdot 1234 = 34$

Conclusion: So first blocking scheme associated with 135, 235, 1234, 12, 524, 154, 34

2 2-way

Example: A 2^5 design can be arranged in 8 blocks of size $2^{5-3} = 4$. Consider two blocking schemes.

1. Define the blocks as

$$B_1 = 135, B_2 = 235, B_3 = 1234.$$

The remaining blocks are confounded with the following interactions:

2. Define the blocks as:

$$B_1 = 12, B_2 = 13, B_3 = 45.$$

Which is a better blocking scheme?

1st better since it associates with less lower-order interaction

Fractional factorial designs

- A 2^k full factorial requires 2^k runs.
- Full factorials are seldom used in practice for large k (k$>=$7).
- For economic reasons fractional factorial designs, which consist of a fraction of full factorial designs are used.

Example - Effect of five factors on six properties of film in eight runs

Five factors were studied in 8 runs (Box, Hunter, and Hunter (2005)). The factors were:

1. Catalyst concentration (A)
2. Amount of additive (B)
3. Amounts of three emulsifiers (C, D, E)

BC is aliased with D
& ABC is aliased with E

Polymer solutions were prepared and spread as a film on a microscope slide. Six different responses were recorded.

BC ABC

run	A	B	C	D	E	y1	y2	y3	y4	y5	y6
1	-1	-1	-1	1	-1	no	no	yes	no	slightly	yes
2	1	-1	-1	1	1	no	yes	yes	yes	slightly	yes
3	-1	1	-1	-1	1	no	no	no	yes	no	no
4	1	1	-1	-1	-1	no	yes	no	no	no	no
5	-1	-1	1	-1	1	yes	no	no	yes	no	slightly
6	1	-1	1	-1	-1	yes	yes	no	no	no	no
7	-1	1	1	1	-1	yes	no	yes	no	slightly	yes
8	1	1	1	1	1	yes	yes	yes	yes	slightly	yes

Example - Effect of five factors on six properties of film in eight runs

$-$
$+$
$-$
$+$
$-$
$+$
$-$
$+$

- The eight run design was constructed beginning with a standard table of signs for a 2^3 design in the factors A, B, C.
- The column of signs associated with the BC interaction was used to accommodate factor D, the ABC interaction column was used for factor E.
- A full factorial for the five factors A, B, C, D, E would have needed $2^5 = 32$ runs.
- Only 1/4 were run. This design is called a quarter fraction of the full 2^5 or a 2^{5-2} design (a two to the five minus two design).
- In general a 2^{k-p} design is a $\frac{1}{2^p}$ fraction of a 2^k design using 2^{k-p} runs.

instead of estimating BC and ABC
we will estimate main effects

Effect Aliasing and Design Resolution

- A chemist in an industrial development lab was trying to formulate a household liquid product using a new process.
- The liquid had good properties but was unstable.
- The chemist wanted to synthesize the product in hope of hitting conditions that would give stability, but without success.
- The chemist identified four important influences: A (acid concentration), B (catalyst concentration), C (temperature), D (monomer concentration).

Effect Aliasing and Design Resolution

- His 8 run fractional factorial design is shown below.

test	A	B	C	D	y
1	-1	-1	-1	-1	20
2	1	-1	-1	1	14
3	-1	1	-1	1	17
4	1	1	-1	-1	10
5	-1	-1	1	1	19
6	1	-1	1	-1	13
7	-1	1	1	-1	14
8	1	1	1	1	10

none of these values are at least 25

- The signs of the ABC interaction is used to accommodate factor D. The tests were run in random order. He wanted to achieve a stability value of at least 25.

Effect Aliasing and Design Resolution

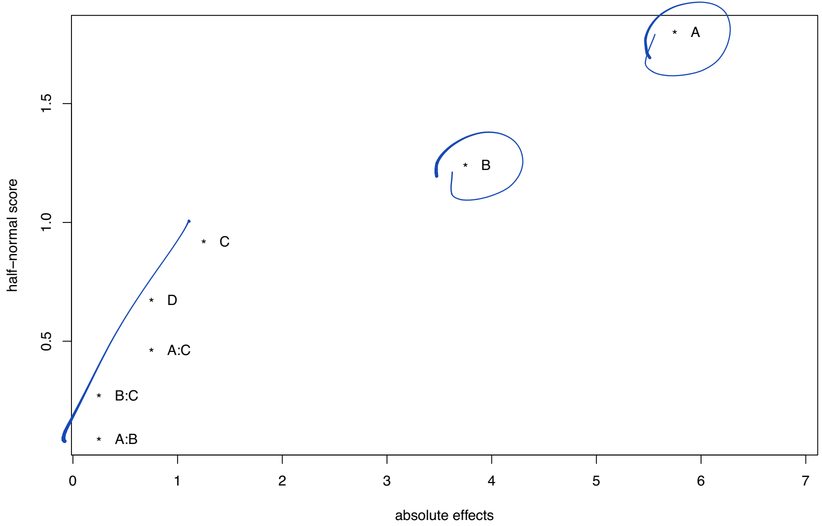
```
fact.prod <- lm(y~A*B*C*D,data=tab0602)
fact.prod1 <- aov(y~A*B*C*D,data=tab0602)
round(2*fact.prod$coefficients,2)
```

```
(Intercept)           A           B           C           D         A:B
      29.25       -5.75       -3.75       -1.25        0.75        0.25
        A:C         B:C         A:D         B:D         C:D       A:B:C
       0.75       -0.25          NA          NA          NA          NA
      A:B:D       A:C:D       B:C:D     A:B:C:D
         NA          NA          NA          NA
```

Even though the stability never reached the desired level of 25, two important factors, A and B, were identified.

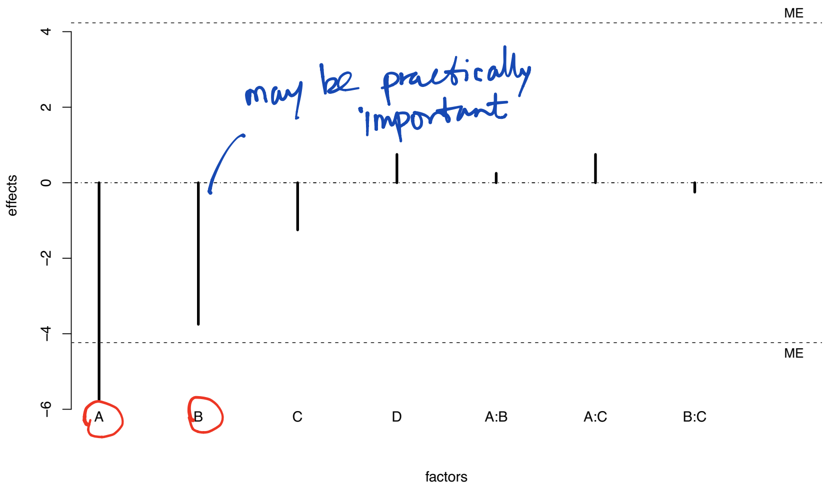
Effect Aliasing and Design Resolution

```
DanielPlot(fact.prod,half = T)
```



Effect Aliasing and Design Resolution

```
LenthPlot(fact.prod1)
```




```
##      alpha       PSE        ME       SME
##   0.050000  1.125000  4.234638 10.134346
```

Effect Aliasing and Design Resolution

What information could have been obtained if a full 2^5 design had been used?

Factors	Number of effects
Main	5
2-factor	10
3-factor	10
4-factor	5
5-factor	1

- 31 degrees of freedom in a 32 run design.
- 16 used for estimating three factor interactions or higher.
- Is it practical to commit half the degrees of freedom to estimate such effects?
- According to effect hierarchy principle three-factor and higher not usually important.
- Thus, using full factorial wasteful. It's more economical to use a fraction of full factorial design that allows lower order effects to be estimated.

Effect Aliasing and Design Resolution

Consider a design that studies five factors in 16 run. A half fraction of a 2^5 or 2^{5-1}.

BCD

16

Run	B	C	D	E	Q
1	-1	1	1	-1	-1
2	1	1	1	1	-1
3	-1	-1	1	1	-1
4	1	-1	1	-1	-1
5	-1	1	-1	1	-1
6	1	1	-1	-1	-1
7	-1	-1	-1	-1	-1
8	1	-1	-1	1	-1
9	-1	1	1	-1	1
10	1	1	1	1	1
11	-1	-1	1	1	1
12	1	-1	1	-1	1
13	-1	1	-1	1	1
14	1	1	-1	-1	1
15	-1	-1	-1	-1	1
16	1	-1	-1	1	1

- The factor E is assigned to the column BCD.
- The column for E is used to estimate the main effect of E and also for BCD.
- The main factor E is said to be **aliased** with the BCD interaction.

Effect Aliasing and Design Resolution

$$E \cdot E = I = BCDE$$

- This aliasing relation is denoted by

$$E = BCD \text{ or } I = BCDE,$$

  where I denotes the column of all $+$'s.
- This uses same mathematical definition as the confounding of a block effect with a factorial effect.
- Aliasing of the effects is a price one must pay for choosing a smaller design.
- The 2^{5-1} design has only 15 degrees of freedom for estimating factorial effects, it cannot estimate all 31 factorial effects among the factors B, C, D, E, Q.

Effect Aliasing and Design Resolution

- The equation $I = BCDE$ is called the **defining relation** of the 2^{5-1} design.
- The design is said to have resolution IV because the defining relation consists of the "word" BCDE, which has "length" 4.
- Multiplying both sides of $I = BCDE$ by column B

$$B = B \times I = B \times BCDE = CDE,$$

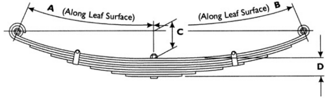
  the relation $B = CDE$ is obtained.
- B is aliased with the CDE interaction. Following the same method all 15 aliasing relations can be obtained.

Effect Aliasing and Design Resolution

- To get the most desirable alias patterns, fractional factorial designs of highest resolution would usually be employed.
- There are important exceptions to this rule that we will not cover in the course.

Example - Leaf spring experiment

An experiment to improve a heat treatment process on truck leaf springs (Wu and Hamada (2009)). The height of the unloaded spring is an important quality characteristic.



Example - Leaf spring experiment

Five factors that might affect height were studied in this 2^{5-1} design.

Factor	Level
B. Temperature	1840 (-), 1880 (+)
C. Heating time	23 (-), 25 (+)
D. Transfer time	10 (-), 12 (+)
E. Hold down time	2 (-), 3 (+)
Q. Quench oil temperature	130-150 (-), 150-170 (+)

Example - Leaf spring experiment

B	C	D	E	Q	y
-1	1	1	-1	-1	7.7900
1	1	1	1	-1	8.0700
-1	-1	1	1	-1	7.5200
1	-1	1	-1	-1	7.6333
-1	1	-1	1	-1	7.9400
1	1	-1	-1	-1	7.9467
-1	-1	-1	-1	-1	7.5400
1	-1	-1	1	-1	7.6867
-1	1	1	-1	1	7.2900
1	1	1	1	1	7.7333
-1	-1	1	1	1	7.5200
1	-1	1	-1	1	7.6467
-1	1	-1	1	1	7.4000
1	1	-1	-1	1	7.6233
-1	-1	-1	-1	1	7.2033
1	-1	-1	1	1	7.6333

Example - Leaf spring experiment

The factorial effects are estimated as before.

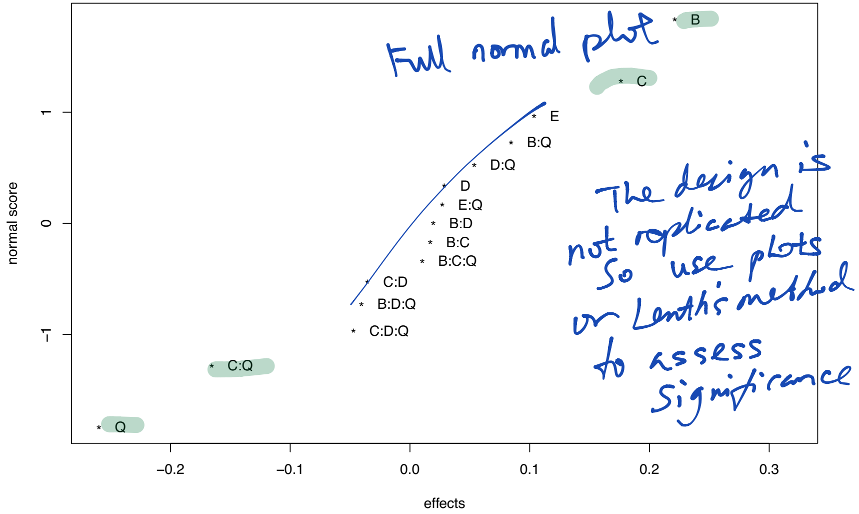
```
library(FrF2)
fact.leaf <- lm(y~B*C*D*E*Q,data=leafspring)
fact.leaf2 <- aov(y~B*C*D*E*Q,data=leafspring)
round(2*fact.leaf$coefficients,2)
```

```
(Intercept)          B          C          D          E          Q
      15.27       0.22       0.18       0.03       0.10      -0.26
        B:C        B:D        C:D        B:E        C:E        D:E
       0.02       0.02      -0.04         NA         NA         NA
        B:Q        C:Q        D:Q        E:Q      B:C:D      B:C:E
       0.08      -0.17       0.05       0.03         NA         NA
      B:D:E      C:D:E      B:C:Q      B:D:Q      C:D:Q      B:E:Q
         NA         NA       0.01      -0.04      -0.05         NA
      C:E:Q      D:E:Q    B:C:D:E    B:C:D:Q    B:C:E:Q    B:D:E:Q
         NA         NA         NA         NA         NA         NA
    C:D:E:Q  B:C:D:E:Q
         NA         NA
```

NA: aliased effects

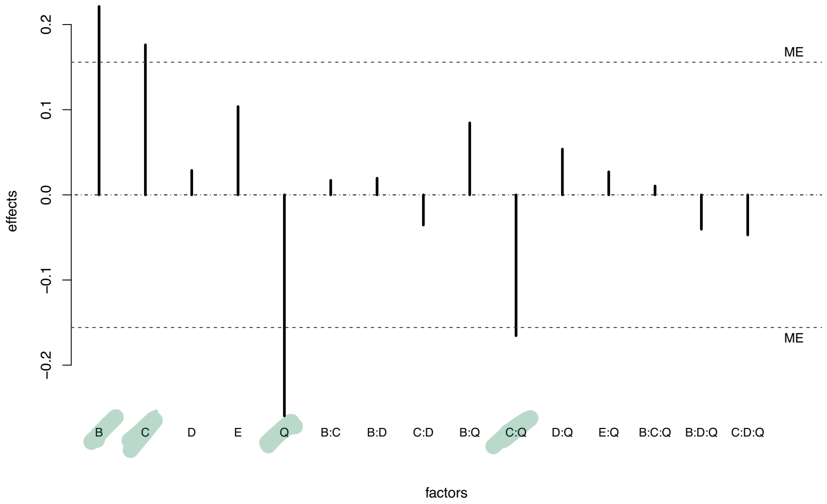
Example - Leaf spring experiment

```
DanielPlot(fact.leaf,half = F)
```



Example - Leaf spring experiment

```
LenthPlot(fact.leaf2,cex.fac = 0.8)
```




```
    alpha       PSE        ME       SME
0.0500000 0.0606000 0.1557773 0.3162503
```