

## STA305/1004-Class 20

March 27, 2017

# 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 defining relations

## Exam review session

I will announce details by the end of the week.

## Example - $2^4$ 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

```
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		

## Half-Normal Plots

- ▶ A related graphical method is called the half-normal probability plot.
- ▶ Let

$$|\hat{\theta}|_{(1)} < |\hat{\theta}|_{(2)} < \dots < |\hat{\theta}|_{(N)}.$$

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

$$|\hat{\theta}|_{(i)} \text{ vs. } \Phi^{-1}(0.5 + 0.5[i - 0.5]/N), i = 1, \dots, N.$$

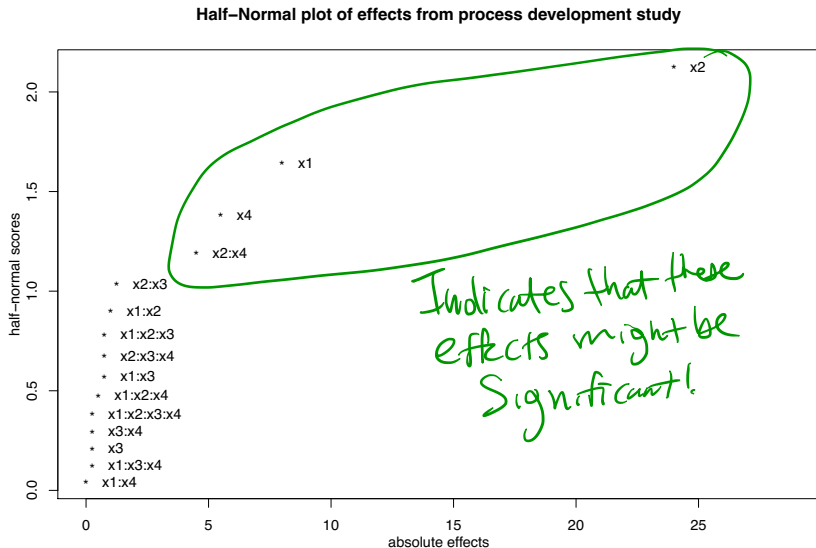
## Half-Normal Plots

- ▶ 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 can be obtained with `DanielPlot()` with the option `half=TRUE`.



## Half-Normal Plots

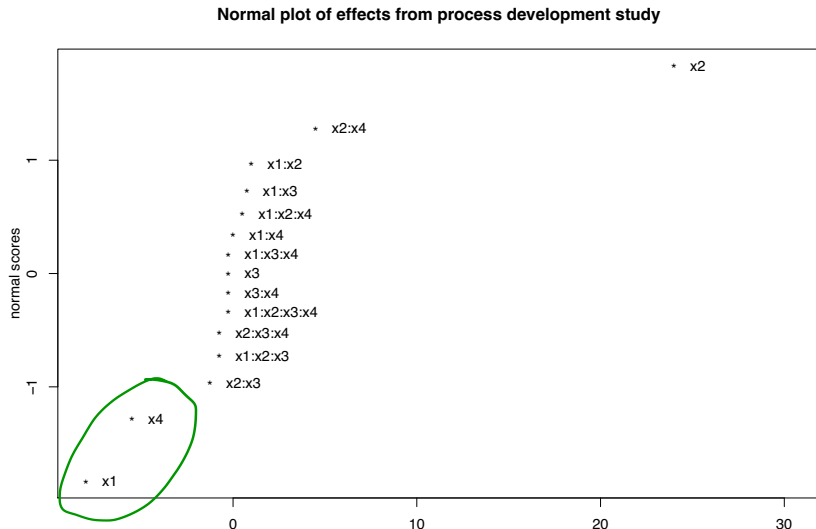
```
library(FrF2)
DanielPlot(fact1, half=TRUE, autolab=F,
           main="Half-Normal plot of effects from process development study")
```



## Half-Normal Plots

Compare with full Normal plot.

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



## Lenth's method: testing significance for experiments without variance estimates

- ▶ Half-normal and normal plots are informal graphical methods involving visual judgement.
- ▶ It's desirable to judge a deviation from a straight line quantitatively based on a formal test of significance.
- ▶ Lenth (1989) proposed a method that is simple to compute and performs well. (ref. pg. 205, Box, Hunter, and Hunter, 2005)

## Lenth's method

- ▶ Let

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

be estimated factorial effects of  $\theta_1, \theta_2, \dots, \theta_N$  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

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

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

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

## 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  $P(|Z| > 2.57) = 0.01, Z \sim N(0, 1)$ .
- ▶  $|\hat{\theta}_i| < 2.5s_0$  trims approximately 1% of the  $\hat{\theta}_i$  if  $\theta_i = 0$ .
- ▶ 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

$$N = 2^k - 1$$

- ▶ 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  $\theta_i$  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,

Bonferroni Correction.

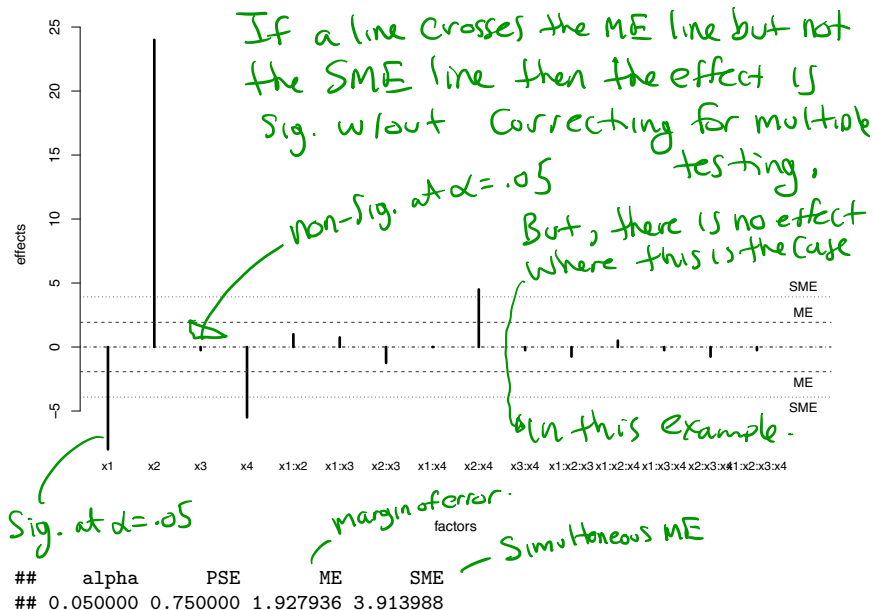
$$SME = t_{d, \gamma} \times PSE,$$

where  $\gamma = (1 + (1 - \alpha)^{1/N}) / 2$ .

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

# Lenth's method - Lenth Plot for process development example

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



## 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

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

$$123 = -$$
$$123 = +$$

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

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.

## 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

$$4.5 = 123 \cdot 23 \\ = 132 \cdot 23 = 13 \cdot 3 = 1$$

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
- ▶ 5 is associated ? 23

## An example of how not to block

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

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

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 separately estimate the main effect 1.
- ▶ Main effects should not be confounded with block effects.



## An example of how not to block

- ▶ 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

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

$$1B_1 = 112 = 2 \text{ and } B_12 = 122 = 122 = 1.$$

- ▶ 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  $B_12$ .

## How to do it

$$4=12$$

$$4 \cdot 4 = 124$$

$$I = 124$$

$I = \text{Column of } +1$

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

Run	45
Block I 2,7	- -
II 3,6	- +
III 4,5	+ -
IV 1,8	+ +

$$124 \cdot 135 = 2345$$

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

— So a better blocking scheme compared to previous

## 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  $B_1, B_2, \dots, B_q$  be the block variables and the factorial effect  $v_i$  is confounded with  $B_i$ ,

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

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

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

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

## Generators and Defining Relations

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

$$7 = 2^3 - 1$$

Consider two blocking schemes.

1. Define the blocks as

$$B_1 B_2 = 12, B_1 B_3 = 245, \\ B_2 B_3 = 145, B_1 B_2 B_3 = 34$$

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

2 - two factor interactions

The remaining blocks are confounded with the following interactions:

2. Define the blocks as:

$$B_1 B_2 = 23, B_1 B_3 = 1245$$

4 - two factor interactions

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

$$B_2 B_3 = 1345$$

$$B_1 B_2 B_3 = 2345$$

Which is a better blocking scheme?

∴ First scheme is better! ∵ Confounds less lower order interactions.