

STA305/1004-Class 19

Nov. 28, 2019

Today's Class

- ▶ Lenth's Method for Assessing significance in unreplicated factorial designs
- ▶ Blocking factorial designs
 - ▶ Effect hierarchy principle
 - ▶ Generation of orthogonal blocks
 - ▶ Generators and defining relations

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

run	x1	x2	x3	x4	conversion
1	-1	-1	-1	-1	70
2	1	-1	-1	-1	60
3	-1	1	-1	-1	89
4	1	1	-1	-1	81
5	-1	-1	1	-1	69
6	1	-1	1	-1	62
7	-1	1	1	-1	88
8	1	1	1	-1	81
9	-1	-1	-1	1	60
10	1	-1	-1	1	49
11	-1	1	-1	1	88
12	1	1	-1	1	82
13	-1	-1	1	1	60
14	1	-1	1	1	52
15	-1	1	1	1	86
16	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

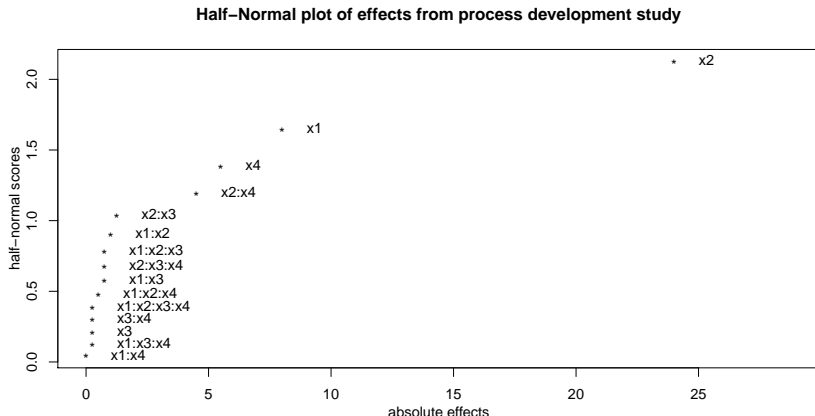
```
fact1 <- lm(conversion~x1*x2*x3*x4,data=tab0510a)
round(2*fact1$coefficients,2)
```

(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

- ▶ 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`.

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



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

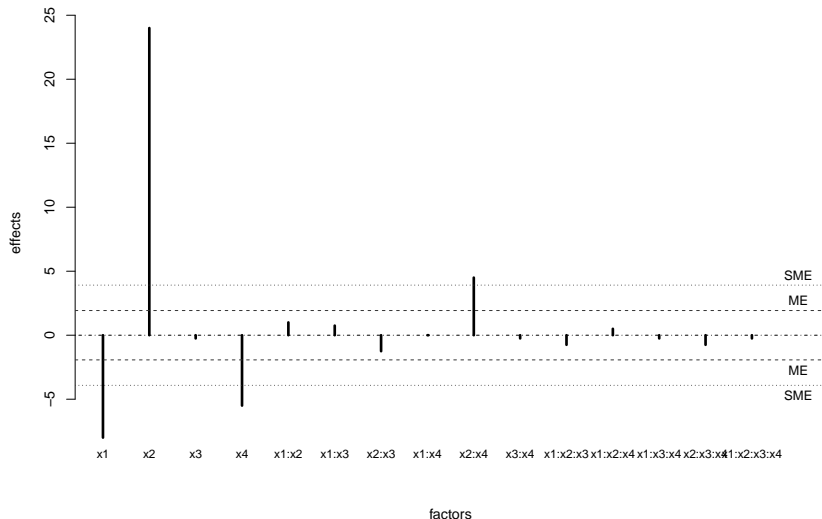
- ▶ Half-normal and normal plots are informal graphical methods involving visual judgement.
- ▶ It's desirable to judge a deviation from a straight line quantitatively based on a formal test of significance.
- ▶ Lenth (1989) proposed a method that is simple to compute and performs well.

Lenth's method

- ▶ Let $\hat{\theta}_{(1)}, \dots, \hat{\theta}_{(N)}$ be $N = 2^k - 1$ factorial effects in a 2^k design.
- ▶ Let m be the median of $|\hat{\theta}|_{(1)}, \dots, |\hat{\theta}|_{(N)}$.
- ▶ An estimate of the standard error of an effect, called the pseudo standard error, is then given by, $s_0 = 1.5m$.
- ▶ Any estimated effect exceeding $2.5s_0$ is excluded, and, if needed m and s_0 are recomputed.
- ▶ A margin of error is then given by $ME = t_{1-\alpha/2, d} \cdot s_0$, where $d = N/3$.
- ▶ All estimates greater than ME may be viewed as “significant”.
- ▶ But, with so many estimates some will be falsely identified.
- ▶ A simultaneous margin of error is: $SME = t_{\gamma, s} \cdot s_0$, where $\gamma = (1 + (1 - \alpha)^{1/N})/2$.
- ▶ Estimated effects exceeding SME are declared significant, but SME is adjusted for multiple comparison.

Lenth's method - Lenth Plot for process development example

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



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

Blocking Factorial Designs

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

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.

Generating Factorial 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 ?
- ▶ 5 is associated ?

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	
II	
III	
IV	

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

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

- ▶ 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?

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 $2^{5-3} = 4$.

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?