TMA4267 Linear Statistical Models V2017 (L19)

Part 4: Design of Experiments
Blocking
Fractional factorial designs

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DOE workflow

1. Set up full factorial design with k factors in R, and
2. randomize the runs.
3. Perform experiments, and enter data into R.
4. Fit a full model (all interactions).
5. If you do not have replications, look at Pareto plots and, use this to suggest at reduced model (if possible). Refit the reduced model.
6. Assess model fit (residual plots, need transformations?).
7. Assess significance.
8. Interpret you results (main and interaction plots).

Q: Randomization

Why do you need to randomize the order in which you perform the experiments?
To make the experiments

- A: random.
- B: robust to external factors.
- C: have constant variance.
- D: independent.

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Genuine run replicates

"When genuine run replicates are made under a given set of experimental conditions, the variation between the associated observations may be used to estimate the standard deviation of the effects. By *genuine* run replicated we mean that variation between runs made at the same experimental conditions is a reflection of the total variability afflicting runs made at different experimental conditions. This point requires careful consideration."

From Box, Hunter, Hunter (1978, 2005): "Statistics for Experimenters", Ch.10.6.

Genuine run replicates

Randomization of run order usually ensures that replicates are genuine. Pilot plant example: each run consists of

1. cleaning the reactor
2. inserting the appropriate catalyst charge
3. running the apparatus at at given temperature and a given feed concentration for 3 hrs to allow the process to settle down at the chosen experimental conditions, and
4. combining chemical analyses made on these samples.

A genuine run replicate must involve the taking of all these steps again. In particular, several chemical analyses from a single run would provide only an estimate of *analytical* variance, usually only a small part of the run-to-run variance.

From Box, Hunter, Hunter (1978, 2005): "Statistics for Experimenters", Ch.10.6.

Pilot plant: A, B and C

A=Temperature, B=Concentration, C=Catalyst, Y=yield.

A	B	C	AB	AC	BC	ABC	Level code	Response
-	-	-	+	+	+	-	1	60
+	-	-	-	-	+	+	a	72
-	+	-	-	+	-	+	b	54
+	+	-	+	-	-	-	ab	68
-	-	+	+	-	-	+	c	52
+	-	+	-	+	-	-	ac	83
-	+	+	-	-	+	-	bc	45
+	+	+	+	+	+	+	abc	80
x_1	x_2	x_3	x_{12}	x_{13}	x_{23}	x_{123}		y

Blocking on ABC

Block 1 consists of experiments with ABC=-1.
Block 2 consists of experiments with ABC=1.

C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	
StdOrder	RunOrder	CenterPt	Blocks	A	B	C	ABC		Y	block effect	
1	1	1	1	-1	-1	-1	-1	1	60	60	
4	4	1	1	-1	1	1	-1	7	45	45	
3	3	1	1	1	-1	1	-1	6	83	83	
2	2	1	1	1	1	-1	-1	4	68	68	
7	7	1	2	-1	-1	1	1	5	52	62	
6	6	1	2	-1	1	-1	1	3	54	64	
5	5	1	2	1	-1	-1	1	2	72	82	
8	8	1	2	1	1	1	1	8	80	90	

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3	3	1	1	1	-1	1	-1	6	83	83
2	2	1	1	1	1	-1	-1	4	68	68
7	7	1	2	-1	-1	1	1	5	52	62
6	6	1	2	-1	1	-1	1	3	54	64
5	5	1	2	1	-1	-1	1	2	72	82
8	8	1	2	1	1	1	1	8	80	90

- ABC is counfunded with the block effect. We can not separate these two effects from eachother.
- Suppose all values in block 2 is increased by 10 units.
  - Then the estimated effect of ABC will increase by 10.
  - But all other estimated effects remain unchanged - and these are the most important to estimate.

Original data

Factorial Fit:
Y versus
Block A B C

Term	Effect	Coef
Constant		64,250
Block		-0,250
A	23,000	11,500
B	-5,000	-2,500
C	1,500	0,750
A*B	1,500	0,750
A*C	10,000	5,000
B*C	0,000	0,000

Added 10 to all obs in Block 2.

Factorial Fit:
"block effect" versus
Block A B C

Term	Effect	Coef
Constant		69,250
Block		-5,250
A	23,000	11,500
B	-5,000	-2,500
C	1,500	0,750
A*B	1,500	0,750
A*C	10,000	5,000
B*C	0,000	0,000

2^3 with four blocks

We need two generators (columns) to define four blocks: the optimal choice is AB and AC

- Block 1: AB=AC=-1 (- -)
- Block 2: AB=-1, AC=1 (- +)
- Block 3: AB=1, AC=-1 (+ -)
- Block 4: AB=AC=1 (+ +)

Std order	A	B	C	AB	AC	BC	ABC
1	-	-	-	+	+	+	-
2	+	-	-	-	-	+	+
3	-	+	-	-	+	-	+
4	+	+	-	+	-	-	-
5	-	-	+	+	-	-	+
6	+	-	+	-	+	-	-
7	-	+	+	-	-	+	-
8	+	+	+	+	+	+	+

2^3 with AB and AC as generators

Std order	A	B	C	AB	AC	BC	ABC	Block
2	+	-	-	-	-	+	+	1
7	-	+	+	-	-	+	-	1
3	-	+	-	-	+	-	+	2
6	+	-	+	-	+	-	-	2
4	+	+	-	+	-	-	-	3
5	-	-	+	+	-	-	+	3
1	-	-	-	+	+	+	-	4
8	+	+	+	+	+	+	+	4

2^3 with AB and AC as generators

- Interaction effects AB and AC are confounded with the block effect, since they are the generators.
- Their product, $AB * AC = A^2BC = BC$, is alco confounded with the block effect (see that BC is constant within each block).
- Adding h_2 to block 2, h_3 to block 3 and h_4 to block 4 does not change the estimated main effects A, B, or C, and not the interaction effect ABC.
- However, AB will change with $2 \cdot h_3 + 2 \cdot h_4 - 2 \cdot h_2$, and we will NOT be able to separate the true AB effect from the block effect.

How to choose which blocks to be used for blocking?

- Idea: try to leave estimates for main effects and low order interaction unchanged by the blocking.
- Note: I=AA=BB=CC, where I is a column of 1's.
- How NOT to do this:
  - Find the blocks for a 2^3 experiment using generators ABC and AC.
  - The interaction between ABC and AC is ABC*AC=B.
  - This means chosing ABC and AC is not a good idea since then we can not trust our estimate of B.

Questions

Should you use a blocking factor in your compulsory project?
Do you understand the difference between blocking and repetition?

Box, Hunter, Hunter: Reactor example

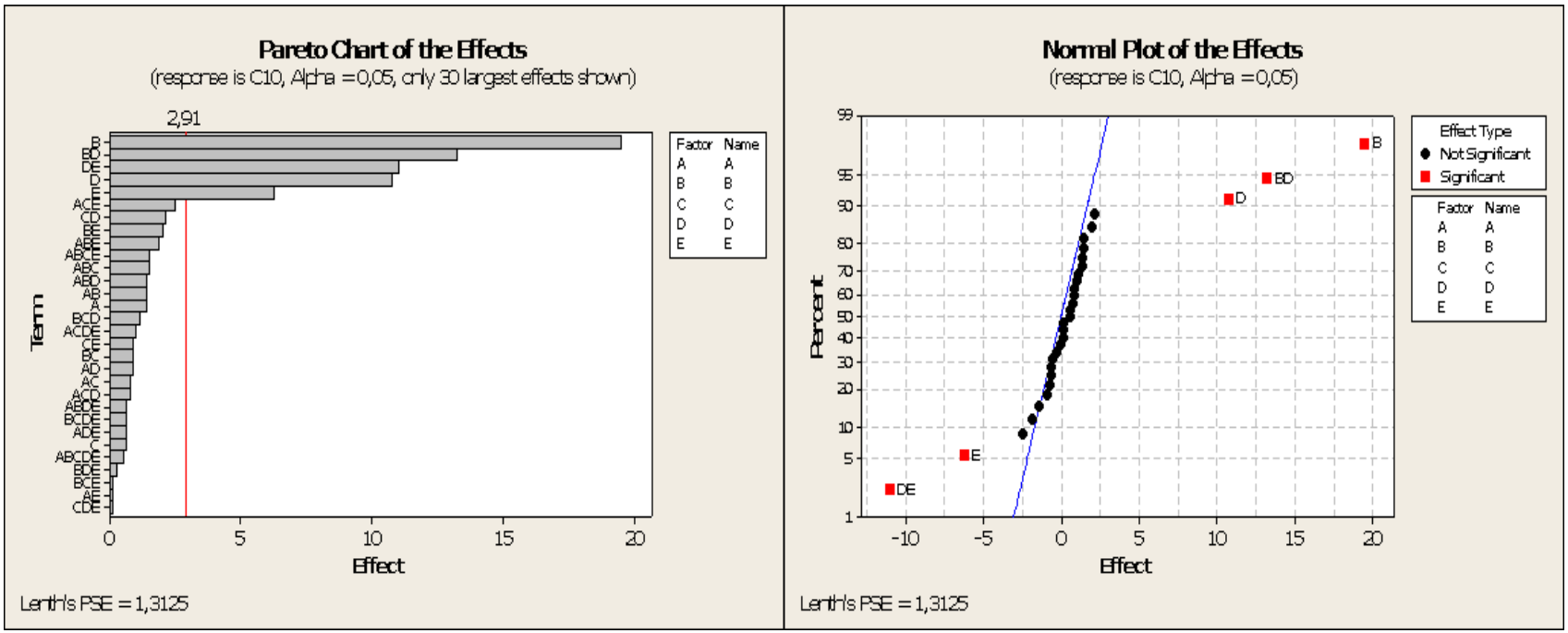
- A=feed rate (liters/min).
- B=Catalyst (%).
- C=Agitation rate (rpm).
- D=Temperature (deg C).
- E=Concentration (%).
- Response= (%) reacted.

Full factorial with $2^5 = 32$ experiments.
From Box, Hunter, Hunter (1978, 2005): "Statistics for Experimenters", Ch.12.2.

Reactor data: standard order

	A	B	C	D	E	y		A	B	C	D	E	y
1	-1	-1	-1	-1	-1	61	17	-1	-1	-1	-1	1	56
2	1	-1	-1	-1	-1	53	18	1	-1	-1	-1	1	63
3	-1	1	-1	-1	-1	63	19	-1	1	-1	-1	1	70
4	1	1	-1	-1	-1	61	20	1	1	-1	-1	1	65
5	-1	-1	1	-1	-1	53	21	-1	-1	1	-1	1	59
6	1	-1	1	-1	-1	56	22	1	-1	1	-1	1	55
7	-1	1	1	-1	-1	54	23	-1	1	1	-1	1	67
8	1	1	1	-1	-1	61	24	1	1	1	-1	1	65
9	-1	-1	-1	1	-1	69	25	-1	-1	-1	1	1	44
10	1	-1	-1	1	-1	61	26	1	-1	-1	1	1	45
11	-1	1	-1	1	-1	94	27	-1	1	-1	1	1	78
12	1	1	-1	1	-1	93	28	1	1	-1	1	1	77
13	-1	-1	1	1	-1	66	29	-1	-1	1	1	1	49
14	1	-1	1	1	-1	60	30	1	-1	1	1	1	42
15	-1	1	1	1	-1	95	31	-1	1	1	1	1	81
16	1	1	1	1	-1	98	32	1	1	1	1	1	82

Pareto and Normal plot



Redundancy

- The number of runs in a full 2^k factorial design increases geometrically when k is increased.
- E.g. $k = 7$ factors gives $2^7 = 128$ runs and we can estimate
  - $\binom{7}{1} = 7$ main effects
  - $\binom{7}{2} = 21$ 2nd order interactions
  - $\binom{7}{3} = 35$ 3rd order interactions
  - $\binom{7}{4} = 35$ 4th order interactions
  - $\binom{7}{5} = 21$ 5th order interactions
  - $\binom{7}{6} = 7$ 6th order interactions
  - $\binom{7}{7} = 1$ 7th order interactions

Redundancy (cont.)

- There is a hierarchy in absolute magnitude: the main effects tend to be larger than the 2nd order interactions, which tends to be larger than the 3rd order interactions, which ...
- At some point higher order interactions tend to become negligible and can be discarded.
- If many factors are introduced into a design, it often happens that some have *no* distinguishable effect at all.
- *Fractional factorial designs* exploit this redundancy!

Full 2^3 factorial experiment

How can we accomodate four factors here?

Std order	A	B	C	AB	AC	BC	ABC
1	-	-	-	+	+	+	-
2	+	-	-	-	-	+	+
3	-	+	-	-	+	-	+
4	+	+	-	+	-	-	-
5	-	-	+	+	-	-	+
6	+	-	+	-	+	-	-
7	-	+	+	-	-	+	-
8	+	+	+	+	+	+	+

Full 2^3 factorial experiment - turned into 4-factor experiment

Which effects are confounded?

	A	B	C	AB	AC	BC	D=ABC	ABD	ACD	BCD	ABCD
1	-	-	-	+	+	+	-	-	-	-	+
2	+	-	-	-	-	+	+	-	-	+	+
3	-	+	-	-	+	-	+	-	+	-	+
4	+	+	-	+	-	-	-	-	+	+	+
5	-	-	+	+	-	-	+	+	-	-	+
6	+	-	+	-	+	-	-	+	-	+	+
7	-	+	+	-	-	+	-	+	+	-	+
8	+	+	+	+	+	+	+	+	+	+	+

Half fraction of 2^4

- The design is called 2^{4-1}_{IV}.
- D=ABC is called the *generator* for the design.
- I=ABCD is called the *defining relation* for the design.
- The design is said to have *resolution IV*.
- The *alias structure* defines which effects are confounded:
  - A+BCD, B+ACD, C+ABD, D+ABC.
  - AB+CD, AC+BD, BC+AD.

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- Should then the block effect be a part of the regression model? (In most cases: yes!)
- Why don't we want to perform a full factorial experiment, but a instead a fractional factorial? (If we have many factors we maybe not need to be able to estimate all possible interactions, and may accept that effects are confounded.)

What did we learn today?

- What is the easiest way to design a half-fraction of a 2^k factorial experiment? (Perform all the experiments where the highest order interaction =-1 or +1. E.g. for k=4 we may do 16 different experiments, and now we only do the 8 possible experiments where ABCD=+1=defining relation. This is the same as thinking that D=ABC=generator).

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- New words: *generator(s)*, *defining relation(s)*, *resolution*.
- Next time: more on interpreting "confounding", interpreting "resolution" and more fractional factorial experiments