NTNU
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TMA4267 Linear Statistical Models V2014 (21)

Design of experiments (note): fractions of 2^k experiments (pages 20-29)

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Box, Hunter, Hunter: Reactor example

— A=feed rate (liters/min).

— B=Catalyst (%).

— C=Agitation rate (rpm).

— D=Temperature (deg C).

— E=Concentration (%).

— Response= (%) reacted.

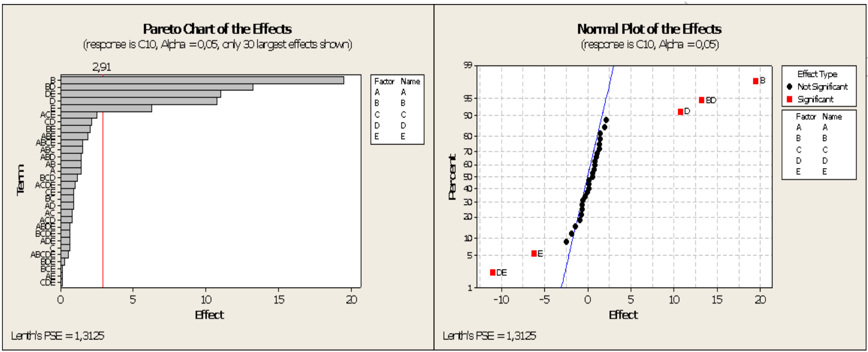
Full factorial with $2^5 = 32$ experiments.

From Box, Hunter, Hunter (1978, 2005): "Statistics for Experimenters", Ch.12.2.

Reactor data: standard order

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

DOE: Fractional factorial design

BH4 Reactor example.

Observation: when the number of factors (k) is large, it may not be optimal to perform a full 2^k factorial design due to the possible redunency of the design.

higher order interactions tend to be smaller than lower order interactions.

Solution: only perform a fraction of the full design

$\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}, \ldots$

Now: we move in the opposite direction to solve this.

We have a full 2^3 factorial design with factors A, B, C; but we also want to have factor D in the experiment. What if we use the ABC column to define the levels of D.

1) D = ABC is called the "generator" of the design.

2) I = D·D = ABCD is called the "defining relation" of the design
(I: column of 1s)
I = ABCD

3) The number of letters (length) of the defining relation is called the "resolution" of the design, denoted by Roman numerals. Here: IV

4) Finally, this is called a half-fraction of a 2^4 design.

NOTATION 2^{4-1}_{IV} design with I = ABCD defining relation

and D = ABC as design generator

We perform 8 experiments, and we may fit 8 parameters

→ this is DOE!

and we use Lenth's method to estimate σ^2.

With 4 factors:

4 main effect A, B, C, D

$\binom{4}{2} = \frac{4 \cdot 3}{2} = 6$ 2-way interactions (AB, AC, ..)

$\binom{4}{3} = \frac{4 \cdot 3 \cdot 2}{3 \cdot 2} = 4$ 3-way interactions (ABC, ABD, ACD, BCD)

$\binom{4}{4} = 1$ 4-way interaction

$\Rightarrow$ $4 + 6 + 4 + 1 = 15$ possible effects (+1 intercept)

Q: what can we estimate?

The "alias" structure defines which effects are confounded.

Obvious: Since $D = ABC$, D and ABC are confounded

$\Rightarrow \hat{D}$ may actually be $\hat{D} + \widehat{ABC}$.

Method: I want to find if any effects are confounded with A.

I multiply A with the defining relation for the design, here: $I = ABCD$

1) Main effect:

$$A = A \cdot I = \underbrace{A \cdot A}_{I} BCD = BCD \quad \Leftrightarrow \quad A = BCD$$

column A and BCD are equal

2) 2-way interactions

$AB = AB \cdot I = ABABCD = CD$ ↑ ? $A^2 = I$, $B^2 = I$

$AC = AC \cdot ABCD = BD$

$AD = AD \cdot ABCD = BC$

$l_{AB} = AB + CD$

$l_{AC} = AC + BD$

$l_{AD} = AD + BC$

3) 3-way interaction term : already known

$l_A = A + BCD$, $l_B = B + ACD$, $l_C = C + ABD$

$l_D = D + ABC$

4) 4-way.

$I = ABCD$, and confounded with the intercept.

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.

We choose D = ABC and got a design of resolution IV.

What if we instead choose D = AB ?

1) D = AB   generator

2) I = ABD   defining relation

3) Resolution: III 2^{4-1}_{III}

Alias pattern:

$A = A \cdot I = A \cdot ABD = BD$

$B = B \cdot ABD = AD$

$C = C \cdot ABD = ABCD$

$D = AB$

We will prefer a resolution IV design to a resolution III design.

Resolution

A design of resolution

- III does not confound main effets with one another, but does confound main effects with two-factor interactions.
- IV does not confound main effects and two-factor interactions, but does confound two-factor interactions with other two-factor interactions.
- V does not confound main effects and two-factor interactions with eachother, but does confound two-factor interactions with three-factor interactions and so on.

In general the resolution of a two-level factional design is *the length of the shortest word in the defining relation*.

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.

Half fraction with reactor example

- Instead of running a full factorial with $2^5 = 32$ experiments,
- we suggest running a half-fraction.
- We choose $I = ABCDE$ as the defining relation.
- Alternative thinking:
  - Construct a full 2^4 design for A, B, C and D.
  - The column of signs for the ABCD interaction is written and used to define the levels for factor E.
  - This means $E = ABCD$ is the generator for the design, and $I = ABCDE$ is the defining relation.
- What is the resolution for this design?
- Write down the aliasing pattern.

Reactor data: standard order

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

Ex: 2^5 half fraction with $E = ABCD$ as design generator and $I = ABCDE$ defining relation.

a) Resolution: V

b) Alias pattern:

$A \cdot ABCDE = BCDE$
B
C
D
E
} main effect & 4-way

$AB \cdot ABCDE = CDE$
⋮
} 2-way & 3-way

$ABC \cdot ABCDE = DE$ ↙

$ABCD$

$ABCDE$ & intercept

Optimal $\frac{1}{2}$ fraction

A half fraction with highest resolution is obtained by

1) Write down a full factorial design in the first $(k-1)$ factors.

2) Associate the kth factor with + or ÷ times the $(k-1)$th factor interaction.

Ex: $k=5$, set-up full 2^4 for A, B, C, D and let $\underbrace{E = ABCD}_{\text{E same sign as ABCD}}$ or $\underbrace{E = -ABCD}_{\text{E opposite sign as ABCD}}$

If we want to set-up a $\frac{1}{4}$ fraction, we need two defining relations, $\frac{1}{8}$ fraction need 3, $\frac{1}{16}$ need 4

Bicycle: 2^{7-4}_{III} ← see slide

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Interpretation of confounding: example

Suppose there are three factors, A, B, C, for which we know the true effects and interaction effects:

$$
\begin{aligned}
A &= 8 \\
B &= 20 \\
C &= 2 \\
AB &= 4 \\
AC &= 2 \\
BC &= 6 \\
ABC &= 4
\end{aligned}
$$

Also is known that average response is 70.

True regression model

The corresponding regression model is:

$$y = \beta_0 + \beta_1 z_1 + \beta_2 z_2 + \beta_3 z_3 + \beta_{12} z_{12} + \beta_{13} z_{13} + \beta_{23} z_{23} + \beta_{123} z_{123} + \epsilon$$

where $z_{12} = z_1 z_2$, $z_{13} = z_1 z_3$, $z_{23} = z_2 z_3$, $z_{123} = z_1 z_2 z_3$, and where the coefficients β are half the corresponding effects, while $\beta_0 = 70$. The regression model is hence

$$y = 70 + 4z_1 + 10z_2 + z_3 + 2z_{12} + z_{13} + 3z_{23} + 2z_{123} + \epsilon$$

In the following we shall also for simplicity assume that the errors ϵ are 0. This makes it possible to compute the responses for any experiment for which the levels of A, B, C are specified.

Confounding example (cont.)

Assume now that a 2^{3-1} experiment is performed, with generator $C = AB$. And responses are computed using the true regression model (check!).

St. order		A	B	C=AB	AB	AC	BC	ABC	y
1	+	-	-	+	+	-	-	+	57
2	+	+	-	-	-	-	+	+	65
3	+	-	+	-	-	+	-	+	73
4	+	+	+	+	+	+	+	+	93
	Const.	z_1	z_2	z_3	z_{12}	z_{13}	z_{23}	z_{123}	
Coeff.	70	4	10	1	2	1	3	2	

Confounding example (cont.)

It is now seen that in all of these 4 experiments are

$$\begin{aligned} Const. &= z_{123} \\ z_1 &= z_{23} \\ z_2 &= z_{13} \\ z_3 &= z_{12} \end{aligned}$$

so for the performed experiment we may as well write the model as

$$y = (\beta_0 + \beta_{123}) + (\beta_1 + \beta_{23})z_1 + (\beta_2 + \beta_{13})z_2 + (\beta_3 + \beta_{12})z_3$$

Using that we know the values of the coefficients, the true model for the data is thus

$$\begin{aligned} y &= (70+2) + (4+3)z_1 + (10+1)z_2 + (1+2)z_3 \\ &= 72 + 7z_1 + 11z_2 + 3z_3 \end{aligned}$$

Confounding example (cont.)

- Suppose now that we try to compute the main effect of A from our data. Apparently this will be

$$\ell_A = \frac{65+93}{2} - \frac{57+73}{2} = 79 - 65 = 14$$

which is also found as twice the coefficient before z_1 in the regression model above.

- Similarly, the apparent interaction effect of B and C would be computed as

$$\ell_{BC} = \frac{-57+65-73+93}{2} = 14$$

The truth (which is known to us) is, however, that $A = 8$ and $BC = 6$, so that it is the sum of A and BC which is 14.

This is what is meant by saying that the main effect of A and the interaction effect between B and C are *confounded* (mixed). The confounded effects are listed in R as the *alias structure*.

```
Factorial Fit: y versus A; B; C


Estimated Effects and Coefficients for y (coded units)


Term      Effect    Coef
Constant           72,000
A         14,000    7,000
B         22,000   11,000
C          6,000    3,000


Alias Structure
I + A*B*C
A + B*C
B + A*C
C + A*B
```

The bicycle example

TABLE 12.5. An eight-run experimental design for studying how time to cycle up a hill is affected by seven variables (I = 124, I = 135, I = 236, I = 1237).

run	seat up/down 1	dynamo off/on 2	handlebars up/down 3	gear low/medium 4 12	raincoat on/off 5 13	breakfast yes/no 6 23	tires hard/soft 7 123	time to climb hill (sec) y
1	−	−	−	+	+	+	−	69
2	+	−	−	−	−	+	+	52
3	−	+	−	−	+	−	+	60
4	+	+	−	+	−	−	−	83
5	−	−	+	+	−	−	+	71
6	+	−	+	−	+	−	−	50
7	−	+	+	−	−	+	−	59
8	+	+	+	+	+	+	+	88

From Box, Hunter, Hunter (1978, 2005): "Statistics for Experimenters", Ch.12.25

The bicycle example

- Set up a full factorial design in the three variables A, B, C.
- Use the generators: D=AB, E=AC, F=BC, G=ABC.
- Defining relations: I=ABD=ACE=BCF=ABCG.
- The design is of resolution III.
- It is a $1/16$ fraction of the full 2^7, and thus called 2_{III}^{7-4}.
- A design where every available contrast is associated with a factor is called a *saturated design*.