Analysis of designs with resolution at least V

- For designs of at least resolution V, all the main effects and two-factor interactions are clear. Then, further decomposition of these effects according to the linear-quadratic system allows all the effects (each with one degree of freedom) to be compared in a half-normal plot. ← if no replicates

  orthogonal component / multi-way layout

  c.f. half-normal plot for orthogonal components

- Note that for effects to be compared in a half-normal plot, they should be uncorrelated and have the same variance. ← use scaling.

  can do t-test if there are replicates.

resolution $\geq V$

model of interest: $y \sim$ all M.E. + all 2fi + ε

← the model matrix is orthogonal (meaning?)

projection onto any 4 factors. → 3^4 full factorial

1. $A, B, C, \cdots, A{\times}B, A{\times}C, \cdots$
2. $A, B, C, \cdots, AB, AB^2, AC, AC^2, \cdots$
3. $A_\ell, A_q, B_\ell, B_q, \cdots, (AB)_{\ell\ell}, (AB)_{\ell q}, (AB)_{q\ell}, (AB)_{qq}, (AC)_{\ell\ell}, \cdots$

Analysis of designs with resolution smaller than V

e.g. III. ME $\xleftrightarrow{\text{alias}}$ 2fi

IV. 2fi $\xleftrightarrow{\text{alias}}$ 2fi

- For designs with resolution III or IV, a more elaborate analysis method is required to extract the maximum amount of information from the data.
- Consider the 3^{3-1} design with $C = AB$ whose design matrix is given in Table 6.

partial aliasing ← effects (1-dim) have correlation $\in [-1, 1]$ ← collinearity in LM.

c.f. Recall: regular design under orthogonal components effects (each 2-dim in 3 levels case): either orthogonal or fully aliased. → correlation $\in \{-1, 1, 0\}$

Table 6: Design Matrix for the 3^{3-1} Design

Run	A	B	C (AB)	AB^2
1	0	0	0	0
2	0	1	1	2
3	0	2	2	1
4	1	0	1	1
5	1	1	2	0
6	1	2	0	2
7	2	0	2	2
8	2	1	0	1
9	2	2	1	0

$A_\ell\, A_q\, B_\ell\, B_q\, C_\ell\, C_q\, (AB)_{\ell\ell} \cdots (AB)_{qq}$ — 4 effect, 4, 4

- Its main effects and two-factor interactions have the aliasing relations:

$I = ABC^2$

$$A = BC^2, B = AC^2, C = AB, \boxed{AB^2 = BC = AC}. \tag{6}$$

Analysis of designs with resolution III (contd)

- In addition to estimating the six degrees of freedom in the main effects A, B and C, there are two degrees of freedom left for estimating the three aliased effects AB^2, BC and AC, which, as discussed before, are difficult to interpret.
- Instead, consider using the remaining two degrees of freedom to estimate any pair of the $l \times l, l \times q, q \times l$ or $q \times q$ effects between A, B and C.
- Suppose that the two interaction effects taken are $(AB)_{ll}$ and $(AB)_{lq}$. Then the eight degrees of freedom can be represented by the model matrix given in Table 7.

d.f.
2 $A=BC^2$
2 $B=AC^2$
2 $C=AB$ ← $A\times B$
2 $AB^2=BC=AC$

1 A_l
1 A_q
1 B_l
1 B_q
1 C_l
1 C_q
1 ← 2 $(AB)_{ll}, (AB)_{lq}, (AB)_{ql}, (AB)_{qq}$

Table 7: A System of Contrasts for the 3^{3-1} Design

$(A)_l \times B_l$; $A_l \times B_q$, $(AB)_{ql}$, $(AB)_{qq}$

Run	A_l	A_q	B_l	B_q	C_l	C_q	$(AB)_{ll}$	$(AB)_{lq}$
1	-1	1	-1	1	-1	1	1	-1
2	-1	1	0	-2	0	-2	0	2
3	-1	1	1	1	1	1	-1	-1
4	0	-2	-1	1	0	-2	0	0
5	0	-2	0	-2	1	1	0	0
6	0	-2	1	1	-1	1	0	0
7	1	1	-1	1	1	1	-1	1
8	1	1	0	-2	-1	1	0	-2
9	1	1	1	1	0	-2	1	1

not orthogonal anymore

identifiable model

exercise: "not" span AB^2 space — $(AB^2)_l$ $(AB^2)_q$

Analysis of designs with resolution III (contd)

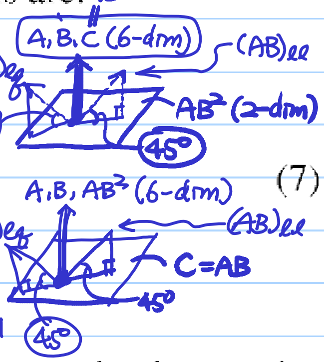
partial aliasing

- Because any component of $A \times B$ is orthogonal to A and to B, there are only four non-orthogonal pairs of columns whose correlations are: AB

complex aliasing — Suppose $y \sim$ all ME + all 2fi + ε.

$A_l, A_q, B_l, B_q, C_l, C_q$,
$(AB)_{ll}, (AB)_{lq}, \cdots$
$(AC)_{ll}, (AC)_{lq}, \cdots$
$(BC)_{ll}, (BC)_{lq}, \cdots$ ← full model is unidentifiable
# of effects $= 1+6+12 = 19 \equiv p$
# of d.f. (9 runs) $= 9 \equiv n$
$\Rightarrow p > n$

$$
\begin{aligned}
Corr((AB)_{ll}, C_l) &= -\sqrt{\tfrac{3}{8}}, \\
Corr((AB)_{ll}, C_q) &= -\tfrac{1}{\sqrt{8}}, \\
Corr((AB)_{lq}, C_l) &= \tfrac{1}{\sqrt{8}}, \\
Corr((AB)_{lq}, C_q) &= -\sqrt{\tfrac{3}{8}}.
\end{aligned} \tag{7}
$$



maximum estimable model (use all d.f.)

- Obviously, $(AB)_{ll}$ and $(AB)_{lq}$ can be estimated in addition to the three main effects.

why? — $(AB^2)_l, (AB^2)_q$ c.f.

① A_l — C_q, $(AB)_{ll}$, $(AB)_{lq}$
② A_l — C_q, $(AC)_{ll}$, $(AC)_{lq}$
③ A_l — B_q, $(AB)_{ll}$, ..., $(AB)_{qq}$
⋮

- Because the last four columns are not mutually orthogonal, they cannot be estimated with full efficiency.

① $cov(\hat\beta) \propto (X^TX)^{-1}$ ② furthermore,
true: $y = X_1\beta_1 + X_2\beta_2 + \varepsilon$
fit: $y = X_1\beta_1 + \varepsilon'$

they have different model matrix

- The estimability of $(AB)_{ll}$ and $(AB)_{lq}$ demonstrates an advantage of the linear-quadratic system over the orthogonal components system. For the same design, the AB interaction component cannot be estimated because it is aliased with the main effect C.

→ regular design (e.g. 2-level case)

one model matrix
$I=ABC$
⑧ $A+B+C$
⑧ $A+B+AB$

Q: can we also decompose the orthogonal component (2-dim) into meaningful 1-dim effect for ?

Analysis Strategy for Qualitative Factors

Ans: dummy variables.

- For a qualitative factor like factor D (lot number) in the seat-belt experiment, the linear contrast $(-1, 0, +1)$ may make sense because it represents the comparison between levels 0 and 2.

← Helmert coding.

- On the other hand, the "quadratic" contrast $(+1, -2, +1)$, which compares level 1 with the average of levels 0 and 2, makes sense only if such a comparison is of practical interest. For example, if levels 0 and 2 represent two internal suppliers, then the "quadratic" contrast measures the difference between internal and external suppliers.

average of all μ with $D=0$ ← $E(y)$

$$\begin{array}{c|cc} D & & \\ \mu_0 \leftarrow 0 & -1 & 1 \\ \mu_1 \leftarrow 1 & 0 & -2 \\ \mu_2 \leftarrow 2 & 1 & 1 \end{array}$$

$$\begin{bmatrix}\mu_0\\ \mu_1\\ \mu_2\end{bmatrix} = \begin{bmatrix}1 & -1 & 1\\ 1 & 0 & -2\\ 1 & 1 & 1\end{bmatrix}\begin{bmatrix}\beta_0\\ \beta_1\\ \beta_2\end{bmatrix} \Rightarrow \underset{\sim}{\beta} = \begin{bmatrix}1/3 & 1/3 & 1/3\\ -1/2 & 0 & 1/2\\ 1/6 & -2/6 & 1/6\end{bmatrix}\begin{bmatrix}\mu_0\\ \mu_1\\ \mu_2\end{bmatrix}$$

$$\beta_2 = \frac{2}{6}\left(\frac{\mu_2+\mu_0-2\mu_1}{2}\right)$$

(*)

$$\begin{array}{c|ccccc} 0 & -1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & 1 & & \vdots \\ 2 & 0 & -2 & 1 & \ddots & \\ \vdots & \vdots & 0 & -3 & & 1 \\ k & 0 & \vdots & \vdots & & -k \end{array}$$

Analysis Strategy for Qualitative Factors (contd)

- When the quadratic contrast makes no sense, two out of the following three contrasts can be chosen to represent the two degrees of freedom for the main effect of a qualitative factor:

Sum coding

$$\begin{bmatrix}\mu_0\\ \mu_1\\ \mu_2\end{bmatrix} = \begin{bmatrix}1 & -1 & -1\\ 1 & 1 & 0\\ 1 & 0 & 1\end{bmatrix}\begin{bmatrix}\beta_0\\ \beta_1\\ \beta_2\end{bmatrix}$$

$$D_{01} = \begin{cases} -1 & \text{for level } 0 \\ 1 & \text{for level } 1 \\ 0 & \text{for level } 2 \end{cases} \text{ of factor } D,$$

D	D_{01}	D_{02}
0	-1	-1
1	1	0
2	0	1

$$\Rightarrow \underset{\sim}{\beta} = \begin{bmatrix}1/3 & 1/3 & 1/3\\ -1/3 & 2/3 & -1/3\\ -1/3 & -1/3 & 2/3\end{bmatrix}\begin{bmatrix}\mu_0\\ \mu_1\\ \mu_2\end{bmatrix}$$

c.f. the (*) in LNp.1-41.

$$\beta_0 = (\mu_0+\mu_1+\mu_2)/3 \equiv \bar{\mu}$$

$$\beta_1 = -\tfrac{1}{3}\mu_0 + \tfrac{2}{3}\mu_1 - \tfrac{1}{3}\mu_2 = \mu_1 - \left(\frac{\mu_0+\mu_1+\mu_2}{3}\right) = \mu_1 - \bar{\mu}$$

$$\beta_2 = \mu_2 - \bar{\mu}$$

$$D_{02} = \begin{cases} -1 & \text{for level } 0 \\ 0 & \text{for level } 1 \\ 1 & \text{for level } 2 \end{cases} \text{ of factor } D,$$

$$\begin{array}{c|cccc} D & & & & \\ 0 & -1 & -1 & \cdots & -1 \\ 1 & 1 & & & 0 \\ 2 & 0 & \ddots & & \\ \vdots & & & & \\ k & 0 & 0 & & 1 \end{array}$$

$D_{02}-D_{01}$ //

$$D_{12} = \begin{cases} 0 & \text{for level } 0 \\ -1 & \text{for level } 1 \\ 1 & \text{for level } 2 \end{cases} \text{ of factor } D,$$

Analysis Strategy for Qualitative Factors (contd)

Note: can only put two out of (D_{01}, D_{02}, D_{12}) into the model.

- Mathematically, they are represented by the standardized vectors:

$$D_{01} = \frac{1}{\sqrt{2}}(-1,1,0), D_{02} = \frac{1}{\sqrt{2}}(-1,0,1), D_{12} = \frac{1}{\sqrt{2}}(0,-1,1).$$

$X^{-1} \neq X^T$

- These contrasts are not orthogonal to each other and have pairwise correlations of $1/2$ or $-1/2$. ↳ why its interpretation different from the Helmert coding (β_2 in sum coding, β_1 in Helmert coding)
- On the other hand, each of them is readily interpretable as a comparison between two of ~~the~~ three levels.
- The two contrasts should be chosen to be of interest to the investigator. For example, if level 0 is the main supplier (reference) and levels 1 and 2 are minor suppliers, then D_{01} and D_{02} should be used. — treatment coding

$\beta_0 = \mu_0,\ \beta_1 = \mu_1 - \mu_0,\ \beta_2 = \mu_2 - \mu_0$

D	D_{01}	D_{02}
0	0	0 ← reference level.
1	1	0
2	0	1

Qualitative and Quantitative Factors

- The interaction between a quantitative factor and a qualitative factor, say $A \times D$, can be decomposed into four effects. ← 1-dim
- As in (5), we define the four interaction effects as follows:

	A	D	A_l	A_q	D_{01}	D_{02}	a	b	c	d
μ_{00} ←	0	0	-1	1	-1	-1	1	1		
μ_{01}	0	1	-1	1	1	0	-1	0		
	0	2	-1	1	0	1	0	-1		
⋮	1	0	0	-2	-1	-1	0	0		
	1	1	0	-2	1	0	0	0		
	1	2	0	-2	0	1	0	0		
	2	0	1	1	-1	-1	1	-1		
	2	1	1	1	1	0	-1	0		
μ_{22}	2	2	1	1	0	1	0	1		

$\begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_8 \end{bmatrix}$

$$\begin{aligned}
a\ (AD)_{l,01}(i,j) &= A_l(i)D_{01}(j), \\
b\ (AD)_{l,02}(i,j) &= A_l(i)D_{02}(j), \\
c\ (AD)_{q,01}(i,j) &= A_q(i)D_{01}(j), \\
d\ (AD)_{q,02}(i,j) &= A_q(i)D_{02}(j).
\end{aligned} \tag{8}$$

D=1 ↔ average | A=0: $\mu_{01} - \frac{\mu_{00}+\mu_{01}+\mu_{02}}{3}$

difference (D=1 ↔ average | A=2): $\mu_{21} - \frac{\mu_{20}+\mu_{21}+\mu_{22}}{3}$

	μ_{00}	μ_{01}	μ_{02}	μ_{10}	μ_{11}	μ_{12}	μ_{20}	μ_{21}	μ_{22}
$a \propto$	1	-2	1	0	0	0	-1	2	-1
$b \propto$	1	1	-2	0	0	0	1	1	-2
$c \propto$	-1	2	1	~~0~~ 2	~~0~~ -4	~~0~~ 2	-1	2	1
$d \propto$	-1	-1	2	2	2	-4	-1	-1	2

$$\underset{\sim}{\beta} = \begin{bmatrix} \beta_0 = 1/9 & \cdots & 1/9 \\ \propto -1\ -1\ -1\ 0\ 0\ 0\ 1\ 1\ 1 \\ \propto 1\ 1\ 1\ -2\ -2\ -2\ 1\ 1\ 1 \\ -1/9\ 2/9\ -1/9\ -1/9\ +2/9\ -1/9\ -1/9\ 2/9\ -1/9 \\ \propto -1\ -1\ 2\ -1\ -1\ 2\ -1\ -1\ 2 \\ \vdots \end{bmatrix} \underset{\sim}{\mu}$$

Variable Selection Strategy

want to solve [non-orthogonality, $p > n$] problem.

choose coding → decompose into 1-dim spaces

Since many of these contrasts are not mutually orthogonal, a general purpose analysis strategy cannot be based on the orthogonality assumption. Therefore, the following variable selection strategy is recommended.

→ Q: how many analyses mentioned in DOE class are based on the assumption?

(i) For a quantitative factor, say A, use A_l and A_q for the A main effect.

(ii) For a qualitative factor, say D, use D_l and D_q if D_q is interpretable; otherwise, select two contrasts from D_{01}, D_{02}, and D_{12} for the D main effect.

(iii) For a pair of factors, say X and Y, use the products of the two contrasts of X and the two contrasts of Y (chosen in (i) or (ii)) as defined in (5) or (8) to represent the four degrees of freedom in the interaction $X \times Y$.

model selection → identify important effects.

a difference between them later need to estimate ?.

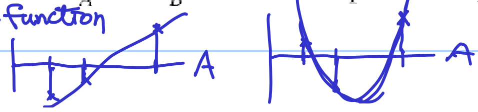
(iv) Using the contrasts defined in (i)-(iii) for all the factors and their two-factor interactions as candidate variables, perform a stepwise regression or subset selection procedure to identify a suitable model. To avoid incompatible models, use the effect heredity principle to rule out interactions whose parent factors are both not significant.

AIC, BIC, PRESS, ...

2nd-order polynomial 1st-order polynomial

(v) If all the factors are quantitative, use the original scale, say x_A, to represent the linear effect of A, x_A^2 the quadratic effect and $x_A^i x_B^j$ the interaction between x_A^i and x_B^j. This works particularly well if some factors have unevenly spaced levels.

base function



Analysis of Seat-Belt Experiment

- Returning to the seat-belt experiment, although the original design has resolution IV, its capacity for estimating two-factor interactions is much better than what the definition of resolution IV would suggest.

total 27 runs.

- After estimating the four (8) main effects, there are still 18 degrees of freedom available for estimating some components of the two-factor interactions.

- From (2), A, B, C and D are estimable and only one of the two components in each of the six interactions $A \times B$, $A \times C$, $A \times D$, $B \times C$, $B \times D$ and $C \times D$ is estimable.

all ME + 2fi: $1 + 4 \times 2 + 6 \times 4 = 33$

$1 + 3 \times 2 + 3 + 3 \times 4 + 3 \times 6 = 40$

- Because of the difficulty of providing a physical interpretation of an interaction component, a simple and efficient modeling strategy that does not throw away the information in the interactions is to consider the contrasts (A_l, A_q), (B_l, B_q), (C_l, C_q) and (D_{01}, D_{02}, D_{12}) for the main effects and the 30 products between these four groups of contrasts for the interactions.

Analysis of Seat-Belt Experiment (contd)

- Using these 39 contrasts as the candidate variables, the variable selection procedure was applied to the data.
- Performing a stepwise regression on the strength data (response y_1), the following model with an R^2 of $\boxed{0.811}$ was identified:

9/27

$$\begin{aligned} \hat{y}_1 &= 6223.0741 + 1116.2859A_l - 190.2437A_q + 178.6885B_l \\ &\quad -589.5437C_l + 294.2883(AB)_{ql} + 627.9444(AC)_{ll} \\ &\quad -191.2855D_{01} - 468.4190D_{12} - 486.4444(CD)_{l,12} \end{aligned} \tag{9}$$

- Note that this model obeys effect heredity. The A, B, C and D main effects and $A \times B$, $A \times C$ and $C \times D$ interactions are significant. In contrast, the simple analysis from the previous section identified the A, C and D main effects and the $AC(=BD^2)$ and $AB(=CD^2)$ interaction components as significant.

LN p.1-26

Analysis of Seat-Belt Experiment (contd)

- Performing a stepwise regression on the flash data (response y_2), the following model with an R^2 of 0.857 was identified:

9/27

$$\begin{aligned} \hat{y}_2 &= 13.6657 + 1.2408A_l + 0.1857B_l \\ &\quad -0.8551C_l + 0.2043C_q - 0.9406(AC)_{ll} \\ &\quad -0.3775(AC)_{ql} - 0.3765(BC)_{qq} - 0.2978(CD)_{l,12} \end{aligned} \tag{10}$$

- Again, the identified model obeys effect heredity. The A, B, and C main effects and $A \times C$, $B \times C$ and $C \times D$ interactions are significant. In contrast, the simple analysis from the previous section identified the A and C main effects and the $AC(=BD^2)$, AC^2 and BC^2 interaction components as significant.

Suggestion: should try to identify more "well-fitted" submodels..

Reading: textbook, 6.6