ST 5203: Experimental Design

(Semester 1, AY 2017/2018)

Text book: Experiments: Planning, Analysis, and Optimization (2nd. edition)

by Jeff Wu and Mike Hamada

Topic 6: Blocking and Confounding

- Fractional Factorial (F.F.) experiments
- From mathematical point of view
- Parcel estimates in F.F.
- Generator, defining contrast subgroup and aliasing relation
- Minimum aberration criterion
- Hidden replication Property
- Techniques for resolving ambiguities in aliased effects
- · Blocking in F.F. design

Motivation of Fractional Factorial Design

In the following, "fi" is an abbreviation of "factor interaction".

• Consider an experiment with 10 factors. A 2^{10} full factorial design needs at least $2^{10}=1024$ runs, with

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10 main effects, 45 2fi's, 120 3fi's, 210 4fi's, 252 5fi's, 210 6fi's, 120 7fi's, 45 8fi's, 10 9fi's, 1 10fi's
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- Using effect hierarchy principle, one would argue that 4fi's, 5fi's, ..., 10 fi's and even 3fi's are not likely to be important. There are $120+210+\ldots+1=968$ such high order interaction effects.
- From informational point of view, every one of the 1024 runs is able to provide the estimate for one parameter (effect), which means 968/1024 = 94.53% of runs are redundant/wasted! Using a full 2^{10} design can be wasteful (unless 1024 runs cost about the same as 1024 968 = 56 runs.)

Notations of 2^{k-p} Design

- Usually, a fractional factorial (F.F.) design is denoted as 2^{k-p} , where
 - k = # of factors.
 - 2 = # levels for each factor.
 - $2^{k-p} = \text{total } \# \text{ of runs.}$
 - $2^{-p} = \text{fraction}$.
- A F.F. requires $2^k/2^p = 2^{k-p}$ number of runs.
- Choosing a F.F. design instead of a full factorial design is usually due to the economic reason.
- When p is large, F.F. saves a lot.

Example: 2³⁻¹ Design

 We start with the a simple example. Recall what we did in the last topic: a 2³ design in 2 blocks. The best scheme is to use ABC as the blocking scheme. In the experiment, what if we perform only those runs for ABC at +?

Treatment	Α	В	С	ABC	Performed runs
(1)	_	_	_	_	
a	+	_	_	+	✓
Ь	-	+	_	+	✓
ab	+	+	_	_	
С	_	_	+	+	✓
ac	+	_	+	_	
bc	-	+	+	_	
abc	+	+	+	+	✓

- Clearly, this is a 2^{3-1} design, where only the runs a, b, c and abc are performed.
- With this experiment, what can we gain and what do we need to pay?

From Mathematical Point of View

 Clearly, we can not estimate all 8 effects, since we only have 4 runs. Let's examine the following regression equations,

$$a = \mu + \frac{A}{2} - \frac{B}{2} - \frac{C}{2} - \frac{AB}{2} - \frac{AC}{2} + \frac{BC}{2} + \frac{ABC}{2}$$

$$b = \mu - \frac{A}{2} + \frac{B}{2} - \frac{C}{2} - \frac{AB}{2} + \frac{AC}{2} - \frac{BC}{2} + \frac{ABC}{2}$$

$$c = \mu - \frac{A}{2} - \frac{B}{2} + \frac{C}{2} + \frac{AB}{2} - \frac{AC}{2} - \frac{BC}{2} + \frac{ABC}{2}$$

$$abc = \mu + \frac{A}{2} + \frac{B}{2} + \frac{C}{2} + \frac{AB}{2} + \frac{AC}{2} + \frac{BC}{2} + \frac{ABC}{2}$$

• 8 parameters versus 4 equations. Certainly unsolvable.

From Mathematical Point of View (Cont.)

 We use the "parcel idea" to explain confounding. Let's "pack" the effects in the following way

$$a = \left(\mu + \frac{ABC}{2}\right) + \frac{1}{2}(A + BC) - \frac{1}{2}(B + AC) - \frac{1}{2}(C + AB)$$

$$b = \left(\mu + \frac{ABC}{2}\right) - \frac{1}{2}(A + BC) + \frac{1}{2}(B + AC) - \frac{1}{2}(C + AB)$$

$$c = \left(\mu + \frac{ABC}{2}\right) - \frac{1}{2}(A + BC) - \frac{1}{2}(B + AC) + \frac{1}{2}(C + AB)$$

$$abc = \left(\mu + \frac{ABC}{2}\right) + \frac{1}{2}(A + BC) + \frac{1}{2}(B + AC) + \frac{1}{2}(C + AB)$$

From Mathematical Point of View (Cont.)

- The solutions of the equations are delivered by parcels, i.e. $\left(\mu + \frac{ABC}{2}\right)$, (A+BC), (B+AC) and (C+AB) can be estimated as four parcels from the regression equations. Unfortunately, no single effect can be estimated correctly!
- More carefully examine the four parcels, the grand mean μ, main effects A, B, C are respectively aliased with 3fi's ABC and 2fi's BC, AC, AB. Use effect hierarchy principle, μ, A, B and C are more likely to be significant. Thus, if we assume ABC, AB, AC and BC are negligible, then we can estimate μ, A, B, C using the parcel estimates.

Estimation of Parcels

- Note the "-" and "+" in the 4 previous equations. They
 consist of the model matrix of a 2² full factorial design
 (explain).
- If we pretend that the 2^2 responses in the 4 previous equations are the responses from a 2^2 full factorial, then the estimated effects can be taken as the parcel estimates of this 2^{3-1} F.F..
- Together with the arguments in the last slide, estimates of μ , A, B, AB by pretending the observations as from the 2^2 full design are, in fact, estimating μ , A, B and C respectively.
- We can rearrange the rows of 4 observations (a, b, c, abc) such that they follow the "standard" order. See the following table.

Estimation of Parcels (Cont.)

	μ	Α	В	С	AB	AC	ВС	ABC	Parcels
С	+	_	_	+	+	_	_	+	$\mu + \frac{ABC}{2}$
а	+	+						1	$A + \overline{BC}$
b	+	_	+	_	_	+	+ -	+	B + AC
abc	+	+	+	+	+	+	+	+	C + AB

- If we check the effects of A and BC, we can see that
 - A and BC are in the parcel (A+BC).
 - The column A and +BC in the above table are exactly the same.
 - If we check the other half of the original 2³ experiment (with the runs (1), ab, ac, bc), then A and BC will still be included in the same parcel, but the parcel becomes (A-BC).
 Meanwhile, the column A will be equal to the column -BC.
- Similar observations for the pairs B and AC, C and AB.
- This does not happen by chance! They are the consequence of the defining relations.

Effect Aliasing, Defining Relation and Generator

 Checking the columns of extracted model matrix in the last slide, we immediately have the column relationships:

$$I = ABC$$
, $A = BC$, $B = AC$, $C = AB$, (1)

which deliver the aliasing relationships: μ is aliased with ABC; A with BC; B with AC; C with AB.

• All relationships in (1) can be summarized in

$$I = ABC. (2)$$

• I = ABC is the defining relation for this 2^{3-1} design. It implies all the three effect aliasing relations:

$$A = BC$$
, $B = AC$, $C = AB$.

• The relation C = AB is called the generator. (explain)



Designing a 2^{k-p} F.F., Generators

- In order to design a 2^{k-p} F.F. with factors $\{A_i : i = 1, ..., k\}$, the experimenter needs to find p independent generators as follows.
 - 1. Separate the k factors into 2 disjoint sets, with one set containing p factors, another containing k-p factors. For the ease of presentation, let's assume the two sets are $\mathcal{L} = \{A_1, \ldots, A_p\}$ and $\mathcal{R} = \{A_{p+1}, \ldots, A_k\}$.
 - 2. For each i = 1, ..., p, the *i*th generator is written as

$$A_i = A_{i_1} \cdots A_{i_J}, \tag{3}$$

with $A_{i_j} \in \mathcal{R}$ for each j = 1, ..., J, $1 \le J < k - p$.

The p equations in (3) are called the generators.

Designing a 2^{k-p} F.F.: Generators (Cont.)

- R is called the set of independent factors, whose elements only appear on the right-hand side of "=" in the generators; whereas L is called the set of dependent factors, whose elements only appear on the left-hand side of "=" in the generators.
- The runs of the experiment are then organized as follows.
 - We have 2^{k-p} runs in total. The k-p factors in $\mathcal R$ form a full factorial design.
 - The experimental conditions for the p factors in \mathcal{L} are completely determined by the generators in each run.

Defining Contrast Subgroup

• In the p generators in (3), we can move A_i to the right-hand side and obtain

$$I = A_i A_{i_1} \cdots A_{i_J}, \tag{4}$$

where $A_i A_{i_1} \cdots A_{i_j}$'s are p independent defining words. Sometimes, the p equations in (4) are also called generators.

- The set formed by multiplications of these p words is called the defining contrast subgroup. It has "2^p - 1 words" + "1 identity element I".
- The defining contrast subgroup is usually written as " $I = \dots = \dots$ ".
- In a 2^{k-p} F.F. design, the number of elements in the defining contrast group is 2^p , including the identity element I. (why?)



Resolution

- Resolution = the shortest word-length among the $2^p 1$ words.
- The resolution of a F.F. design is usually written in Roman numerals I, II, III, IV, V, ...
- All the aliasing relationships can be derived from the defining contrast subgroup.
- If the generators are given, or if the defining contrast subgroup is given, then the F.F. design is totally determined.

Clear Effects

- A main effect (m.e.) or two-factor interaction effect (2fi) is called clear, if it is not aliased with any other m.e.'s or 2fi's.
- A m.e. or 2fi is called strongly clear if it is not aliased with any other m.e.'s, 2fi's or 3fi's.
- Therefore a clear effect is estimable under the assumption that 3-factor and all higher order interactions are negligible. Likewise, a strongly clear effect is estimable under the weaker assumption that 4-factor and all higher order interactions are negligible.

Clear Effects (Cont.)

• Examples: in the 2^{5-1} design, consider the following two possible generators,

Generators	Resolution	Clear	Strongly Clear
I = BCDE	IV	B, C, D, E	A, AB, AC, AD, AE
I = ABCDE	V	All 10 2fi's	All 5 main effects

• I = ABCDE is better than I = BCDE, because each of the m.e.'s and 2fi's are either clear or strongly clear. Usually, for a 2^{k-1} design, with factors A_1, \ldots, A_k , $I = A_1A_2 \ldots A_k$ is the best design, because (i) it has the maximum resolution k; (ii) each main effect is aliased with a word of length k-1, and each 2fi's is aliased with a word of length k-2.

Example: 2⁵⁻² Design

We start with assigning generators:

$$D = ABC$$
, $E = AB$.

- Defining contrast subgroup is given by
 I = ABCD = ABE = CDE. CDE is obtained by the multiplication of ABCD and ABE.
- The resolution of the design is III.
- Each aliasing relation is derived by the multiplication on all terms of the defining contrast subgroup
 I = ABCD = ABE = CDE.
- All the aliasing relations for m.e.'s and 2fi are derived in the next slide. There are no clear effects and strongly clear effects.

2⁵⁻² Design, Deriving Aliasing Relations

$$A = BCD = BE = ACDE$$
 $B = ACD = AE = BCDE$
 $C = ABD = ABCE = DE$
 $D = ABC = ABDE = CE$
 $E = ABCDE = AB = CD$
 $AB = CD = E = ABCDE$
 $AC = BD = BCE = ADE$
 $AD = BC = BDE = ACD$
 $BC = AD = ACE$
 $BC = AD = ACE = BDE$
 $BD = AC = ADE = BCE$
 $BD = AC = ADE = BCD$
 $CD = AB = ABCDE = E$
 $CE = ABDE = ABC = D$
 $DE = ABCE = ABD = C$

Wordlength Pattern and Resolution

- Define n_i = number of defining words of length i in defining contrast subgroup. $W = (n_3, n_4, n_5, ...)$ is called the wordlength pattern. In the 2^3 design above, W = (2, 1). We usually require a F.F. to have $n_2 = 0$. (why? otherwise, one main effect is aliased with another main effect.)
- Resolution = smallest r such that $n_r \ge 1$. Usually, we include the resolution in the subscript of 2^{k-p} , i.e. $2^{k-p}_{\text{resolution}}$. For example, in the 2^3 design above with generator I = ABCD = ABE, we can write it as 2^{5-2}_{II} .
- Maximum resolution criterion: For fixed k and p, choose a 2^{k-p} design with maximum resolution.

Rules for Resolution

- III: there is no guarantee that there exist clear effects; main effects can be estimated by assuming those 2 or higher order interactions aliased with m.e.'s are negligible.
- IV: all main effects are clear.
- V: all main effects are strongly clear and all two-factor interactions are clear.
- Among the resolution IV designs with given k and p, those with the largest number of clear two-factor interactions are the best.
- Usually, VI, VII, ... are not recommended in real applications for economic reason. So the most commonly used resolutions are III, IV, and V.

Minimum Aberration Criterion

• Motivating example: consider the two 2^{7-2} designs:

design
$$1(d_1)$$
: $I = DEFG = ABCDF = ABCEG$, design $2(d_2)$: $I = ABCF = ADEG = BCDEFG$

Both have resolution IV, but

$$W(d_1) = (0, 1, 2, 0, 0)$$
 and $W(d_2) = (0, 2, 0, 1, 0)$.

Which one is better? Intuitively, one would argue that d_1 is better, because $n_4(d_1) = 1 < 2 = n_4(d_2)$. (Why? Effect hierarchy principle.)

• This is similar to the minimum aberration criterion used in blocking 2^k design in the last topic.

Minimum Aberration Criterion (Cont.)

- For two 2^{k-p} designs, denoted as d_1 and d_2 , let r be the smallest integer such that $n_r(d_1) \neq n_r(d_2)$. Then d_1 is said to have less aberration than d_2 if $n_r(d_1) < n_r(d_2)$. Usually, the smaller aberration, the better.
- If there is no design with less aberration than d_1 , then d_1 has the minimum aberration.
- Minimum aberration criterion can be adopted to select F.F. designs. In the previous 2^{7-2} F.F. design, it can be shown that the generators in d_1 gives the minimum aberration among all 2^{7-2} F.F. designs.

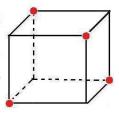
Projection Property: An Example

• Example: consider 2_{III}^{3-1} design with generator C=-AB, then I=-ABC. Take a look at the following cubic.

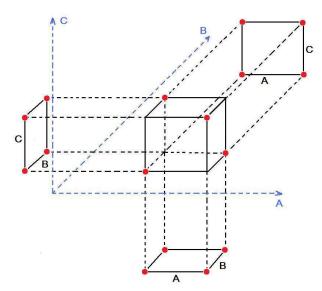
```
y A B C

(1) - - -
ac + - + A = -BC
bc - + + B = -AC
ab + + - AB = -C
```

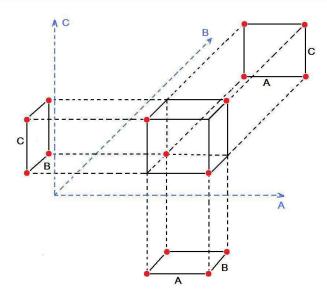
Choose any two factors, we can squeeze the design to be a 2² full factorial of these two chosen factors. In the meanwhile, if we assume the third factor as inert, then all effects of the two chosen factors can be estimated. See the next slide for a better intuitive explanation.



The Case I = -ABC



The Case I = ABC



Use of Design Tables

- The F.F. design table is given in Appendix 5A after Chapter 5. Minimum aberration designs are given in the table.
- 1. Any design given in the table can be immediately extended to 2^p designs. For example, the 2_{III}^{7-4} design has 16 choices

$$D = \pm AB, E = \pm AC, F = \pm BC, G = \pm ABC.$$
 (5)

- The design can possibly be further extended to other designs by exchanging the roles of any two factors. For instance, replace D with A in the above example will lead to another 16 choices of designs.
- Randomly choose any one of the design in real application if no prior preference.

Use of Design Tables (Cont.)

- However, in practice, if specific treatment combinations are deemed undesirable, they can be avoided by choosing a F.F. design that does not contain them using arguments 1 and 2 in the last slide.
- For example, if (+,+,+) for factors A, C, D need to be avoided, can we obtain desirable design only based upon (5)? The answer is no.
- One possible way to solve this problem is to exchange the roles of B and C, say consider the following set of designs:

$$D = \pm AC$$
, $E = \pm AB$, $F = \pm BC$, $G = \pm ABC$.

• Clearly, in order to avoid A, C, D combinations (+,+,+) in the experiment, now we only need to avoid using D=AC in our generator.

Techniques for Resolving Ambiguities in Aliased Effects

- Revisit our 2_{III}^{5-2} design example, I = ABCD = ABE = CDE. If we assume 2fi's and higher order interactions are negligible, all main effects can be estimated.
- However, none of effects are clear, besides, all 2fi's cannot be estimated since they are either aliased with some other 2fi's or main effect.
- The following are three types of techniques that can resolve the ambiguities in a F.F. experiment.
 - Scientific knowledge may suggest that some effects in the aliased set are not likely to be significant.
 - Use effect hierarchy principle to assume some higher order effects are negligible.
 - Use a follow-up experiment to **de-alias** these effects.

Example: Yield of Peanut Oil Experiment

Kligo (1988) reported a 2^{5-1} experiment to determine the effects of the factors listed below on the yield (y) of peanut oil per batch. Based on the data on the next slide, we want to determine the significant factor effects and interactions and fit the corresponding predictive model. By inspection we readily see that the defining relation of this design is I = -ABCDE. Thus the design is of resolution V.

	Le	vel
Factor	_	+
A: CO ₂ pressure (bars)	415	550
B: Temperature ($^{\circ}$ C)	25	95
C: Moisture (% by weight)	5	15
D: Flow (L/min)	40	60
E: Particle Size (mm)	1.28	4.05

Example: Yield of Peanut Oil Experiment (Cont.)

y: Percentage of yield of peanut oil

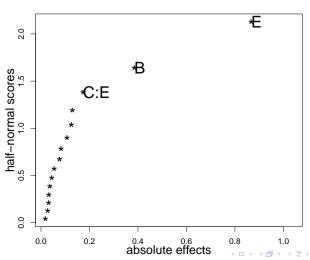
Treatment	Yield	Treatment	Yield
Combination	(%)	Combination	(%)
(1)	63	de	23
ae	21	ad	74
be	36	bd	80
ab	99	abde	33
ce	24	cd	63
ac	66	acde	21
bc	71	bcde	44
abce	54	abcd	96

We use log(y) as the response, because the residual plot for using y directly as a response shows heteroscedasticity.

Example: Yield of Peanut Oil Experiment (Cont.)

Half normal plot with $\alpha = 0.1$.

Half Normal Plot for log.yield, alpha=0.1



Example: Yield of Peanut Oil Experiment (Cont.)

The half normal plot indicates that we can fit a simpler model with only the effects of E, B, CE. The result is summarized in the following table.

Source	D.F.	S.S.	M.S.	F	p value
В	1	0.5950	0.5950	26.834	0.0002
Ε	1	3.0093	3.0093	135.724	0.0000
CE	1	0.1207	0.1207	5.444	0.0378
Error	12	0.2661	0.0222		
Total	15	3.9910			

The fitted model is

$$\widehat{\log y} = 3.8893 + 0.1928x_2 - 0.4337x_5 + 0.0869x_3x_5,$$

where the subscripts "1, 2, 3, 4, 5" correspond to "A, B, C, D, E".

Fold-over Technique: Version I

• Consider a 2_{III}^{7-4} design with generators:

$$d_1: D = AB, E = AC, F = BC, G = ABC$$

None of its main effects are clear.

 In order to de-alias all main effects, examine a follow-up design. Perform another 8 runs (runs 9-16 in Table [2]) with reversed signs for each of the 7 factors. The follow-up design d₂ has generators:

$$d_2: D = -AB, E = -AC, F = -BC, G = ABC$$

- The combined design $d_1 + d_2$ is a 2_{IV}^{7-3} design and thus all main effects are clear. Refer to the next page.
- Note: in Table [2], there is another factor H added. It serves as a block factor to model the possible difference between runs 1-8 and runs 9-16, since they are performed in distinct time periods.

Fold-over Technique: Contrast Subgroups

• For d_1 , its defining contrast subgroup has 8 words of odd length and 7 words of even length:

$$I = ABD = ACE = AFG = BCF = BEG = CDG = DEF = ABCDEFG$$

= $ABCG = ABEF = ACDF = ADEG = BCDE = BDFG = CEFG$

• For d_2 , its contrast subgroup contains 8 odd length words obtained by changing the sign of each odd length word in d_1 and 7 words of even length, which are the same as those in d_1 :

$$I = -ABD = -ACE = -AFG = -BCF = -BEG$$

= $-CDG = -DEF = -ABCDEFG$
= $ABCG = ABEF = ACDF = ADEG = BCDE = BDFG = CEFG$

• The defining contrast subgroup of d (= $d_1 + d_2$) is (explain)

$$I = ABCG = ABEF = ACDF = ADEG = BCDE = BDFG = CEFG$$



[2]: Augmented Model Matrix and Design Matrix

Run	Α	В	С	D = AB	E = AC	F = BC	G = ABC	Н
1	_	_	_	+	+	+	_	+
2	+	_	_	_	_	+	+	+
3	_	+	_	_	+	_	+	+
4	+	+	_	+	_	_	_	+
5	_	_	+	+	_	_	+	+
6	+	_	+	_	+	_	_	+
7	_	+	+	_	_	+	_	+
8	+	+	+	+	+	+	+	+
D	Λ							
Run	-A	-B	-C	-D	-E	-F	-G	
9	-A +	$\frac{-B}{}$	<u>-c</u>	<u>–</u> <i>– –</i>	<u>-Е</u>	<u>-</u> г	— G +	_
					— E — +			
9		+	+	_	_	— г — — +		
9 10 11 12	+ -	+	+ +	+	_			
9 10 11 12 13	+ -	+	+ +	+	+		+	
9 10 11 12	+ - + -	+	+ +	+	- + - +		+	
9 10 11 12 13	+ - + -	+	+ +	+	- + - +		+	

Fold-over Technique: Version II

- Suppose that one factor, say *E*, is very important. We want to de-alias *E* and all 2fi's involving *E*.
- Examine the follow-up 2_{III}^{7-4} design:

$$d_3: D = AB, E = -AC, F = BC, G = ABC,$$

In the follow-up experiment, we reverse only the sign of factor E, while the other factors are kept unchanged. See Table [3].

• The combined design d_1+d_3 continue to be a 2_{III}^{7-3} design, but with generators:

$$d': D = AB, F = BC, G = ABC.$$
 (6)

Since E does not appear in (6). E is strongly clear and all 2fi's involving E are clear. However, there is no guaranteed improvements for other effects.

• For real application, d_2 or d_3 is chosen depending on scientific interests.

[3]: Augmented Model Matrix and Design Matrix

Run	Α	В	С	D = AB	E = AC	F = BC	G = ABC	Н
1	_	_	_	+	+	+	_	+
2	+	_	_	_	_	+	+	+
3	_	+	_	_	+	_	+	+
4	+	+	_	+	_	_	_	+
5	_	_	+	+	_	_	+	+
6	+	_	+	_	+	_	_	+
7	_	+	+	_	_	+	_	+
8	+	+	+	+	+	+	+	+
Run	Α	В	С	D	-E	F	G	
	/ ·	$\boldsymbol{\mathcal{D}}$	C		_	•	U	
9	_	_	_	+	_	+	_	_
	- +	_ _ _	_ _ _		_ +			_
9	_	_ _ _ +	_ _ _ _		_	+	_	_ _ _
9 10	_	_	_ _ _ _		_	+	- +	
9 10 11	- + -	- - +	- - - +		- + -	+	- +	
9 10 11 12	- + -	- - +	- - - + +	+ - - +	- + - +	+	- + +	
9 10 11 12 13	- + - + -	- - +	- - - + +	+ - - +	- + - +	+	- + +	