

Blocking in multi-stage experiments

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Abstract

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In the talk, I will develop some general principles for good design, along with methods for evaluating competing designs.

Example 1 (Treatments orthogonal to blocks in both stages): the problem

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Treatment factor F has 2 levels, which are applied in Stage 1, and these can be changed within each batch.

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Treatment factor G has 3 levels, which are applied in Stage 2, and these can be changed within each lot.

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How should we design the experiment?

Example 1: design 1a

Design 1a Align batches with lots, and allocate the 6 combinations of levels of F and G in a randomized complete-block design.

	G1	G2	G3
F1	a	b	c
F2	d	e	f

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F2	<i>d</i>	<i>e</i>	<i>f</i>

<i>a</i>	<i>a</i>	<i>e</i>	<i>b</i>	<i>c</i>	<i>d</i>
<i>c</i>	<i>b</i>	<i>f</i>	<i>c</i>	<i>d</i>	<i>e</i>
<i>d</i>	<i>f</i>	<i>d</i>	<i>e</i>	<i>a</i>	<i>c</i>
<i>b</i>	<i>e</i>	<i>b</i>	<i>a</i>	<i>f</i>	<i>f</i>
<i>f</i>	<i>c</i>	<i>c</i>	<i>d</i>	<i>b</i>	<i>a</i>
<i>e</i>	<i>d</i>	<i>a</i>	<i>f</i>	<i>e</i>	<i>b</i>

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a	a	e	b	c	d
c	b	f	c	d	e
d	f	d	e	a	c
b	e	b	a	f	f
f	c	c	d	b	a
e	d	a	f	e	b

units		treatments		
source	df	source	df	EMS
Mean	1	Mean	1	$6\sigma_B^2 + 6\sigma_L^2 + \sigma^2 + q_0$
Blocks	5			$6\sigma_B^2 + 6\sigma_L^2 + \sigma^2$
Units[B]	30	F	1	$\sigma^2 + q(F)$
		G	2	$\sigma^2 + q(G)$
		$F\#G$	2	$\sigma^2 + q(FG)$
		residual	25	σ^2

σ^2 = variance of experimental units

σ_B^2 = variance of batches σ_L^2 = variance of lots

$q(F)$ = positive semi-definite quadratic form in parameters for levels of F

Example 1: design 1b

Design 1b Cross batches with lots to form a square array, and allocate the 6 combinations of levels of F and G in a Latin square.

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<i>a</i>	<i>f</i>	<i>b</i>	<i>c</i>	<i>e</i>	<i>d</i>
<i>f</i>	<i>d</i>	<i>a</i>	<i>e</i>	<i>b</i>	<i>c</i>
<i>c</i>	<i>e</i>	<i>f</i>	<i>d</i>	<i>a</i>	<i>b</i>
<i>d</i>	<i>a</i>	<i>c</i>	<i>b</i>	<i>f</i>	<i>e</i>
<i>b</i>	<i>c</i>	<i>e</i>	<i>f</i>	<i>d</i>	<i>a</i>
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c	e	f	d	a	b
d	a	c	b	f	e
b	c	e	f	d	a
e	b	d	a	c	f

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We have lost 5 residual degrees of freedom, and gained nothing.

Lesson

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Brien, Harch, Correll and Bailey (2011) call this “confounding big with big”.

Example 2 (Treatments not orthogonal to blocks): the problem

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In Stage 1, these must be processed in 15 batches of size 4.

There are 10 treatments, which are applied in Stage 1,
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Example 2 (Treatments not orthogonal to blocks): the problem

There are 60 experimental units.

In Stage 1, these must be processed in 15 batches of size 4.

There are 10 treatments, which are applied in Stage 1,
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In Stage 2, the units must be processed in 10 lots of size 6.

No further treatment factor is applied in Stage 2.

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How should we design the experiment?

Example 2: the intuitive part

In Stage 1 we can use a balanced incomplete-block design.

This means that

every pair of treatments occur together in the same number (two) of batches,
and the average variance of the estimators of treatment differences is minimized.

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E	H	F	H	J	I	J	I	C	J	C	G	D	G	I
C	A	B	G	E	F	B	C	I	A	G	C	E	B	A
H	F	E	J	I	H	D	H	J	F	J	D	I	D	G

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E	H	F	H	J	I	J	I	C	J	C	G	D	G	I
C	A	B	G	E	F	B	C	I	A	G	C	E	B	A
H	F	E	J	I	H	D	H	J	F	J	D	I	D	G

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A	B	C	E	F	G	H	D	B	D	A	F	A	E	B
E	H	F	H	J	I	J	I	C	J	C	G	D	G	I
C	A	B	G	E	F	B	C	I	A	G	C	E	B	A
H	F	E	J	I	H	D	H	J	F	J	D	I	D	G

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E	H	F	H	J	I	J	I	C	J	C	G	D	G	I
C	A	B	G	E	F	B	C	I	A	G	C	E	B	A
H	F	E	J	I	H	D	H	J	F	J	D	I	D	G

Use each **row** as a lot in Stage 2.

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A	B	C	E	F	G	H	D	B	D	A	F	A	E	B
E	H	F	H	J	I	J	I	C	J	C	G	D	G	I
C	A	B	G	E	F	B	C	I	A	G	C	E	B	A
H	F	E	J	I	H	D	H	J	F	J	D	I	D	G

Use each row as a lot in Stage 2.

The treatment information lost to lots is the same as the information lost to rectangles, which is part of the information already lost to batches, so no further information is lost in Stage 2.

A surprising lesson

Lesson

*In a nested row-column design,
if the rows within each rectangle have exactly the same treatments
then the loss of information on treatment differences is the same
as it is in the block design obtained by ignoring rectangles and rows.*

This was shown independently by Bagchi, Mukhopadhyay and Sinha (1990), Chang and Notz (1990), and Morgan and Uddin (1993).

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In Example 2, the best design for Stage 2 alone cannot be arranged as a nested row-column design with this property.

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Principle

*If treatments are applied only in Stage 1,
plan the design by starting with the stage in which the block size is smaller.*

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$F1$	$F2$	$F2$	$F1$	$F1$	$F2$
1	3	2	1	1	3
2	2	2	3	2	2
1	1	3	3	2	2
3	3	1	2	1	1
3	1	3	1	3	3
2	2	1	2	3	1

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2	2	2	3	2	2	2	1	2	2
1	1	3	3	2	2	2	3	2	2
3	3	1	2	1	1	1	1	1	1
3	1	3	1	3	3	3	3	3	3
2	2	1	2	3	1	3	3	1	1

units		treatments		
source	df	source	df	EMS
Mean	1	Mean	1	$6\sigma_B^2 + 6\sigma_L^2 + \sigma^2 + q_0$
Blocks	5	F	1	$6\sigma_B^2 + 6\sigma_L^2 + \sigma^2 + q(F)$
		residual	4	$6\sigma_B^2 + 6\sigma_L^2 + \sigma^2$
Units[B]	30	G	2	$\sigma^2 + q(G)$
		$F\#G$	2	$\sigma^2 + q(FG)$
		residual	26	σ^2

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1	3	2	1	1	3				
2	2	2	3	2	2				
1	1	3	3	2	2				
3	3	1	2	1	1				
3	1	3	1	3	3				
2	2	1	2	3	1				

units		treatments		EMS
source	df	source	df	
Mean	1	Mean	1	$6\sigma_B^2 + 6\sigma_L^2 + \sigma^2 + q_0$
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The variance for the contrast between levels of F involves σ_L^2 as well as σ_B^s , so it is larger than it needs to be.

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						units		treatments			
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1	3	2	1	1	3	Mean	1	Mean	1	$6\sigma_B^2 + 6\sigma_L^2 + \sigma^2 + q_0$	
2	2	2	3	2	2	Blocks	5	F	1	$6\sigma_B^2 + 6\sigma_L^2 + \sigma^2 + q(F)$	
1	1	3	3	2	2			residual	4	$6\sigma_B^2 + 6\sigma_L^2 + \sigma^2$	
3	3	1	2	1	1	Units[B]	30	G	2	$\sigma^2 + q(G)$	
3	1	3	1	3	3			$F\#G$	2	$\sigma^2 + q(FG)$	
2	2	1	2	3	1			residual	26	σ^2	

The variance for the contrast between levels of F involves σ_L^2 as well as σ_B^s , so it is larger than it needs to be.

There are 4 residual degrees of freedom for testing the main effect of F , and this cannot be increased.

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F_2	F_1	F_2	F_1	F_1	F_2
1	3	2	3	2	1
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1	1	3	2	3	2
2	3	2	3	1	1
2	2	1	1	3	3

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		residual	4	$6\sigma_B^2 + \sigma^2$
Lots	5			$6\sigma_L^2 + \sigma^2$
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3	2	3	1	1	2
1	1	3	2	3	2
2	3	2	3	1	1
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Main effect of F has smaller variance than before, and same df.

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source	df	source	df	EMS
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Batches	5	F	1	$6\sigma_B^2 + \sigma^2 + q(F)$
		residual	4	$6\sigma_B^2 + \sigma^2$
Lots	5			$6\sigma_L^2 + \sigma^2$
B#L	25	G	2	$\sigma^2 + q(G)$
		$F\#G$	2	$\sigma^2 + q(FG)$
		residual	21	σ^2

Main effect of F has smaller variance than before, and same df.

Other treatment effects have same (small) variance,

Example 3: design 3b

Design 3b Cross batches with lots to form a square array; allocate the 2 levels of F to whole batches, allocate the 3 levels of G to two units in each row and column, and then randomize rows and columns.

F2	F1	F2	F1	F1	F2
1	3	2	3	2	1
3	1	1	2	2	3
3	2	3	1	1	2
1	1	3	2	3	2
2	3	2	3	1	1
2	2	1	1	3	3

units		treatments		
source	df	source	df	EMS
Mean	1	Mean	1	$6\sigma_B^2 + 6\sigma_L^2 + \sigma^2 + q_0$
Batches	5	F	1	$6\sigma_B^2 + \sigma^2 + q(F)$
		residual	4	$6\sigma_B^2 + \sigma^2$
Lots	5			$6\sigma_L^2 + \sigma^2$
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Main effect of F has smaller variance than before, and same df.

Other treatment effects have same (small) variance, and df reduced from 26 to 21.

Principle

If a treatment factor has to be applied to large units such as blocks in one stage, then try to make it orthogonal to blocks in other stages.

Some principles

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If a treatment factor has to be applied to large units such as blocks in one stage, then it will have relatively few residual degrees of freedom.

*In order not to reduce these further,
try to confound the whole of this block term with the same term in other stages.*

Example 3: design 3c

Design 3c Make 3 squares of size $(2 \times 2)/3$ by crossing pairs of batches (shown as rows) with pairs of lots (shown as columns).

<i>F1</i>	<i>G1, G2, G3</i>	<i>G1, G2, G3</i>						
<i>F2</i>	<i>G1, G2, G3</i>	<i>G1, G2, G3</i>						
			<i>F1</i>	<i>G1, G2, G3</i>	<i>G1, G2, G3</i>			
			<i>F2</i>	<i>G1, G2, G3</i>	<i>G1, G2, G3</i>			
						<i>F1</i>	<i>G1, G2, G3</i>	<i>G1, G2, G3</i>
						<i>F2</i>	<i>G1, G2, G3</i>	<i>G1, G2, G3</i>

Randomize levels of *F* to rows within each square;
randomize levels of *G* within each corner of each square.

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						<i>F2</i>	<i>G1, G2, G3</i>	<i>G1, G2, G3</i>

Randomize levels of F to rows within each square;
randomize levels of G within each corner of each square.

Remark Squares is the **supremum** of Batches and Lots:
Squares = Batches \vee Lots.

Example 3: skeleton anova for design 3c

units		treatments		
source	df	source	df	EMS
Mean	1	Mean	1	$6\sigma_B^2 + 6\sigma_L^2 + \sigma_1^2 + q_0$
Squares	2			$6\sigma_B^2 + 6\sigma_L^2 + \sigma_1^2$
Batches[S]	3	F	1	$6\sigma_B^2 + \sigma_1^2 + q(F)$
		residual	2	$6\sigma_B^2 + \sigma_1^2$
Lots[S]	3			$6\sigma_L^2 + \sigma_1^2$
B#L[S]	3			σ_1^2
Units[B,L,S]	24	G	2	$\sigma^2 + q(G)$
		F#G	2	$\sigma^2 + q(FG)$
		residual	20	σ^2

The randomization argument suggests that $\sigma_1^2 \neq \sigma^2$.

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Both residual df have decreased, and nothing has been gained.

Example 4 (Treatment factors confounded with blocks in different stages): the problem

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In Stage 1, these must be processed in 6 batches of size 6.

Treatment factor F has 2 levels, which are applied in Stage 1,
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How should we design the experiment?

Example 4: design 4

Design 4 Cross batches with lots to form a square array; randomize the 2 levels of F to whole batches, randomize the 3 levels of G to whole lots.

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Any further blocking of either batches or lots reduces the already-small residual df for main effects.

More general numbers

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Stage 1 groups them into b batches of size s ;
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with each intersection containing Nm/bc experimental units,

where m divides b , m divides c and bc divides Nm ,

so m divides $\gcd\{b, c\}$, and $\gcd\{b, c\}$ divides $Nm/\text{lcm}\{b, c\}$.

Example 5: calculating possible rectangle sizes

There are 36 experimental units.

In Stage 1, these must be processed in 12 batches of size 3.

In Stage 2, the units must be processed in 9 lots of size 4.

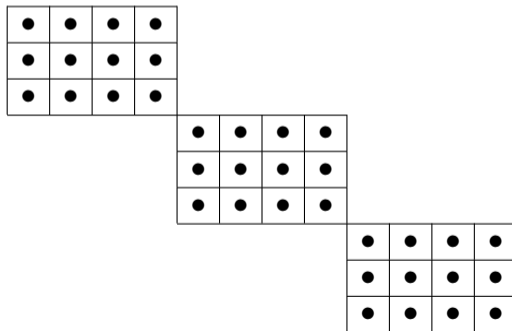
Example 5: calculating possible rectangle sizes

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For orthogonality, the only possibility is three 3×4 rectangles.



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$$s\sigma_B^2 + k\sigma_L^2 + \sigma^2,$$

so these $m - 1$ degrees of freedom are typically not used for inference or estimation.

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It is desirable to keep m small.

Powers of the same small prime

Suppose that the number of batches and the number of lots are both powers of p , where $p = 2$ or $p = 3$, that several p -level treatment factors F_1, F_2, \dots must be applied to whole batches in Stage 1, and several p -level treatment factors G_1, G_2, \dots must be applied to whole lots in Stage 2.

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For example, if $p = 2$, there are 64 experimental units, and F_1, F_2, F_3 and F_4 are applied to 16 whole batches in Stage 1 while G_1, G_2 and G_3 are applied to 8 whole lots in Stage 2, we can use two 4×8 rectangles, and confound $F_1F_2F_3F_4$ and $G_1G_2G_3$ with each other and with rectangles.

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This technique is called **post-fractionation** by Bisgaard (1997) and Vivacqua and Bisgaard (2009).

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- ▶ if a treatment factor is neither orthogonal to blocks nor confounded with them, in both Stages 1 and 2, then a nested row-column design may have surprisingly good properties.