Multi-phase experiments: from design to analysis
Session 2: Non-orthogonality

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An experiment in incomplete blocks

9 Detergents

12 People
3 Laundry-loads in P

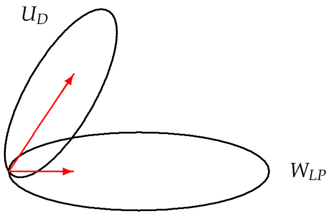
1	4	7	1	2	3	1	2	3	1	2	3
2	5	8	4	5	6	5	6	4	6	4	5
3	6	9	7	8	9	9	7	8	8	9	7

This block design

- is binary, because no treatment occurs more than once in any block;
- has the property that treatment contrasts are not orthogonal to the blocks subspace so we say that the design is not orthogonal;
- is balanced, which means that every pair of distinct treatments occur together in the same number of blocks.

A geometric interpretation of balance

	Experimental units			Treatments	
Subspaces	W_0	W_P	W_{LP}	U_0	U_D
Projectors	$\mathbf{Q}_0$	$\mathbf{Q}_P$	$\mathbf{Q}_{LP}$	$\mathbf{R}_0$	$\mathbf{R}_D$



Every vector in the treatments subspace U_D makes the same angle θ with stratum W_{LP}.
Equivalently, $\mathbf{R}_D\mathbf{Q}_{LP}\mathbf{R}_D = (\cos^2\theta)\mathbf{R}_D$.
$\cos^2\theta$ is called the canonical efficiency factor for U_D in W_{LP}.

A statistical interpretation of balance

In a balanced incomplete-block design with v treatments in blocks of size k,

$$\text{canonical efficiency factor for within-blocks stratum} = \frac{v}{v-1}\,\frac{k-1}{k}.$$

If a treatment contrast is estimated using only within-blocks information, then its variance is inflated by a factor of 1/c.e.f. compared to an unblocked design of the same size with the same stratum variance.

$$\mathbf{R}_D\mathbf{Q}_0 = \mathbf{0} \quad \text{so} \quad \mathbf{R}_D\mathbf{Q}_P\mathbf{R}_D = \mathbf{R}_D - \mathbf{R}_D\mathbf{Q}_{LP}\mathbf{R}_D = (1-\cos^2\theta)\mathbf{R}_D$$

so the canonical efficiency factor for between-blocks stratum = 1 − canonical efficiency factor for within-blocks stratum.

Show this information in the skeleton anova table

plots Ω		treatments Γ		
source	df	cef	source	df
Mean	1	1	Mean	1
People	11	1/4	Detergents	8
			Residual	3
Laundry[People]	24	3/4	Detergents	8
			Residual	16

This table summarizes the properties of the design.
If the difference between two treatments is estimated using only information in W_{LP} then its variance is

$$\frac{2}{\text{replication}} \times \frac{1}{\text{cef}} \times \text{stratum variance} = \frac{2}{4} \times \frac{4}{3} \times \eta_{LP}.$$

Using only information in W_P, the variance is

$$\frac{2}{4} \times \frac{4}{1} \times \eta_P.$$

Strategies for estimation of treatment differences

plots Ω		treatments Γ		
source	df	cef	source	df
Mean	1	1	Mean	1
People	11	1/4	Detergents	8
			Residual	3
Laundry[People]	24	3/4	Detergents	8
			Residual	16

1. Use only information in W_{LP}.
2. Use only information in W_P.
3. Do both the above, estimate η_{LP} and η_P from the residual mean squares, and calculate the minimum-variance unbiased linear combination.
4. Iterate the above, estimating η_{LP} and η_P from the actual residuals at the previous step.
5. Use REML.

A square lattice design

16 Treatments

3 Fields
4 Blocks in F
4 Plots in B, F

1	2	3	4
5	6	7	8
9	10	11	12
13	14	15	16

A	*B*	*C*	*D*
B	*A*	*D*	*C*
C	*D*	*A*	*B*
D	*C*	*B*	*A*

Field 1

1	5	9	13
2	6	10	14
3	7	11	15
4	8	12	16

Field 2

1	2	3	4
5	6	7	8
9	10	11	12
13	14	15	16

Field 3

1	2	3	4
6	5	8	7
11	12	9	10
16	15	14	13

Canonical efficiency factors

1	2	3	4
5	6	7	8
9	10	11	12
13	14	15	16

A	*B*	*C*	*D*
B	*A*	*D*	*C*
C	*D*	*A*	*B*
D	*C*	*B*	*A*

Field 1

1	5	9	13
2	6	10	14
3	7	11	15
4	8	12	16

Field 2

1	2	3	4
5	6	7	8
9	10	11	12
13	14	15	16

Field 3

1	2	3	4
6	5	8	7
11	12	9	10
16	15	14	13

Treatment contrasts between rows of the first array are estimated in Plots[Blocks[Fields]] in only 2 out of 3 fields, so have cef 2/3. Ditto treatment contrasts between columns; treatment contrasts between letters.
Treatment contrasts orthogonal to these have cef 1.

Treatment subspaces

The space of treatment contrasts splits into two orthogonal parts.

Subspace	T_1	T_2
dimension	9	6
cef in P[B[F]]	2/3	1
cef in B[F]	1/3	0
cef in F	0	0

plots Ω		treatments Γ		
source	df	cef	source	df
Mean	1	1	Mean	1
Fields	2			
Blocks[Fields]	9	1/3	T_1	9
Plots[Blocks[Fields]]	36	2/3	T_1	9
		1	T_2	6
			Residual	21

Silly randomization

We choose a design, then randomize it by applying a suitable permutation to the set of plots.

Suppose that the 16 treatments are a 4^2 factorial. Should we randomize the actual treatments to the labels $1, \ldots, 16$?

1. No. Decide whether you want the more precisely estimated contrasts to be both main effects or part of the interaction, and stick with that.
2. No. If the subspaces T_1 and T_2 are not compatible with the breakdown into main effects and interaction, some software may produce strange results.

General block designs

In general, we need to find the eigenspaces of

$$\mathbf{R}_{\text{treatmentcontrasts}}\mathbf{Q}_{\text{Plots[Blocks]}}\mathbf{R}_{\text{treatmentcontrasts}}.$$

The corresponding eigenvalues are the canonical efficiency factors.
These subspaces are not always easy to explain in terms of factors.

A rectangular lattice design

20 Treatments

3 Fields
5 Blocks in F
4 Plots in B, F

	19	14	9	4
5		20	15	10
6	1		16	11
12	7	2		17
18	13	8	3	

A	*C*	*E*	*B*	*D*
E	*B*	*D*	*A*	*C*
D	*A*	*C*	*E*	*B*
C	*E*	*B*	*D*	*A*
B	*D*	*A*	*C*	*E*

Field 1

4	5	1	2	3
9	10	6	7	8
14	15	11	12	13
19	10	16	17	18

Field 2

5	1	2	3	4
6	7	8	9	10
12	13	14	15	11
18	19	20	16	17

Field 3

1	2	3	4	5
8	9	10	6	7
15	11	12	13	14
17	18	19	20	16

Less obvious treatment subspaces

Now it is less easy to describe the three treatment eigenspaces.

Subspace	T_1	T_2	T_3
dimension	7	4	8
cef in P[B[F]]	1	5/6	7/12
cef in B[F]	0	1/6	5/12
cef in F	0	0	0

plots Ω		treatments Γ		
source	df	cef	source	df
Mean	1	1	Mean	1
Fields	2			
Blocks[Fields]	12	1/6	T_2	4
		5/12	T_3	8
Plots[Blocks[Fields]]	45	1	T_1	7
		5/6	T_2	4
		7/12	T_3	8
			Residual	26

Optimality criteria

In an incomplete-block design with canonical efficiency factors $\lambda_1, \ldots, \lambda_{v-1}$ put

$$A = \text{harmonic mean of } \lambda_1, \ldots, \lambda_{v-1}$$
$$E = \text{minimum of } \lambda_1, \ldots, \lambda_{v-1}.$$

Average variance of estimator of treatment difference =

$$\frac{2}{\text{replication}} \times \frac{1}{A} \times \eta_{PB}.$$

Maximum variance of estimator of normalized treatment contrast =

$$\frac{1}{E} \times \eta_{PB}.$$

Both are bounded above by the value for a balanced incomplete-block design with the same parameters.

How good are our designs?

Square lattice design for 16 treatments in 12 blocks of size 4:

$$A = 0.769$$
$$E = 0.669$$
$$\text{BIBD bound} = 0.800$$

This is known to be A-optimal, even over non-resolved designs.

Rectangular lattice design for 20 treatments in 15 blocks of size 4:

$$A = 0.745$$
$$E = 0.583$$
$$\text{BIBD bound} = 0.789$$

You can do a little better by using non-resolved designs.

How does this generalize to more strata? I

Given the treatment subspaces U_i,
with their orthogonal projectors $\mathbf{R}_i$,
and the strata W_j, with their orthogonal projectors $\mathbf{Q}_j$,
what can happen?

If the strata can be labelled such that

$$\mathbf{R}_i\mathbf{Q}_j = \mathbf{0}$$

for all i and for all $j \geq 3$,
then only strata W_1 and W_2 have any information about treatment contrasts,
and the situation is similar to that for incomplete-block designs.

How does this generalize to more strata? II

1. If every treatment subspace U_i is contained in a single stratum W_j then the design is orthogonal.
2. If $\mathbf{R}_i$ commutes with $\mathbf{Q}_j$ for all i and j, then the treatment subspaces U_i can be decomposed into subspaces $U_i \cap W_j$, and this makes the design orthogonal.
   It may be possible to do this by using pseudofactors.
3. If $\mathbf{R}_i\mathbf{Q}_j\mathbf{R}_i = \lambda_{ij}\mathbf{R}_i$ and $\mathbf{R}_i\mathbf{Q}_j\mathbf{R}_k = \mathbf{0}$ for all i, j, k with $k \neq j$ then we have structure balance, and the approach for incomplete-block designs generalizes.
4. If $\mathbf{R}_i\mathbf{Q}_j\mathbf{R}_i$ commutes with $\mathbf{R}_i\mathbf{Q}_m\mathbf{R}_i$ for all i, j and m and $\mathbf{R}_i\mathbf{Q}_j\mathbf{R}_k = \mathbf{0}$ for all i, j, k with $k \neq j$ then each U_i can be decomposed into the common eigenspaces of the $\mathbf{R}_i\mathbf{Q}_j\mathbf{R}_i$, and this makes the design structure-balanced.
5. If $(\sum_i \mathbf{R}_i)\,\mathbf{Q}_j\,(\sum_i \mathbf{R}_i)$ commutes with $(\sum_i \mathbf{R}_i)\,\mathbf{Q}_m\,(\sum_i \mathbf{R}_i)$ for all j and m, then V_Γ can be decomposed into their common eigenspaces, which may not be compatible with the U_i.
6. Otherwise, this approach does not work.

An example with three effective strata

49 Varieties	4 Fields 7 Rows in F 7 Columns in F

Write the 49 varieties in a 7×7 square array; write out a complete set of six mutually orthogonal 7×7 Latin squares.

Field	Field rows	Field columns
1	array rows	array columns
2	letters of LS 1	letters of LS 2
3	letters of LS 3	letters of LS 4
2	letters of LS 5	letters of LS 6

Skeleton anova with three effective strata

Subspace	T_1	T_2
dimension	24	24
cef in R#C[F]	3/4	3/4
cef in R[F]	1/4	0
cef in C[F]	0	1/4
cef in F	0	0

plots Ω		treatments Γ		
source	df	cef	source	df
Mean	1	1	Mean	1
Fields	3			
Rows[Fields]	24	1/4	T_1	24
Columns[Fields]	24	1/4	T_2	24
R#C[Fields]	144	3/4	T_1	24
		3/4	T_2	24
			Residual	96