The Theory of Designed Experiments

8. Blocking

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Blocking

When patterns of likely variation among units are identified, the units are grouped into *blocks* of similar units. Units within a block should be as near homogeneous as possible.

Examples

- In field, glasshouse, or some laboratory, experiments units which are close together in space might form a block.
- In laboratory or industrial experiments units which are close together in time might form a block.
- In animal experiments, animals from the same litter might form a block.
- In clinical trials, patients with similar ages might form a block.

Blocking

The initial definition of blocks is based entirely on the knowledge about the units. The number of treatments to be used is not relevant.

Sometimes there is flexibility, e.g. field experiments, sometimes there is little, e.g. animal experiments.

Information from blocked experiments

The objective of blocking is to get more precise comparisons of treatments by eliminating differences between blocks from the estimated treatment comparisons.

Since the information from the units within blocks stratum is by far the most important, we will design experiments to maximize this information.

Most of the information for comparing treatments comes from comparing treatments which are in the same block (e.g. paired samples t-test).

Example

Compare 6 treatments in 2 blocks, each of 5 units.

Block	
I	II
1	1
2	2
3	3
4	4
5	6

$$(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' =$$

$$\begin{bmatrix}
. & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . \\
-0.5 & 0.5 & 0 & 0 & 0 & -0.5 & 0.5 & 0 & 0 & 0 \\
-0.5 & 0 & 0.5 & 0 & 0 & -0.5 & 0 & 0.5 & 0 & 0 \\
-0.5 & 0 & 0 & 0.5 & 0 & -0.5 & 0 & 0 & 0.5 & 0 \\
-0.625 & -0.125 & -0.125 & -0.125 & 1 & -0.375 & 0.125 & 0.125 & 0.125 & 0 \\
-0.375 & 0.125 & 0.125 & 0.125 & 0 & -0.625 & -0.125 & -0.125 & -0.125 & 1
\end{bmatrix}$$

Obtaining blocked designs

Example: In a variety trial, 6 varieties have to be compared. The field has been split up into 6 blocks of 4 plots each. How should varieties be allocated to the blocks?

In the randomized complete block design, treatment comparisons are *orthogonal* to block effects because each treatment appears equally often in each block. Since $\mathbf{X}'\mathbf{X}$ is then block-diagonal, there is no loss of information, i.e. all information on treatment comparisons appears in the units stratum.

In incomplete block designs treatment comparisons are not orthogonal to block effects. The designs should be chosen to be as nearly orthogonal as possible, so that as much of the information on the important treatment comparisons as possible appears in the units stratum.

Unstructured treatments

If all pairwise comparisons are of interest, then each treatment should appear as near as possible equally often in each block.

Another useful property is balance. A design is *balanced* if all pairs of treatments can be compared equally precisely.

In designs with equally sized blocks balance is achieved when each pair of treatments occur together in blocks equally often. Such designs are called *balanced incomplete block (BIB)* designs.

Unstructured treatments

If a BIB design is not available, the design should be chosen to be as nearly balanced as possible. This implies that

- each pair of treatments should appear together in blocks as near as possible equally often;
- if some treatments appear more often, pairwise concurrences of these treatments with each other, and to a lesser extent with other treatments, should be greater.
- because of indirect comparisons, if pairwise concurrences of one treatment with each of two others are high, pairwise concurrences of these two others need not be high.

Efficiency factors

The efficiency of estimation of a comparison, $\mathbf{c}'\mathbf{t}$, in a blocked design can be measured by its *efficiency factor*:

$$EF(\widehat{\mathbf{c}'\mathbf{t}}) = \frac{V_u(\widehat{\mathbf{c}'\mathbf{t}})/\sigma_u^2}{V(\widehat{\mathbf{c}'\mathbf{t}})/\sigma^2},$$

where the subscript u denotes the equivalent unblocked design. $V(\widehat{\mathbf{c}'\mathbf{t}})/\sigma^2$ is obtained from $\mathbf{X}'\mathbf{X}^{-1}$ and $V_u(\widehat{\mathbf{c}'\mathbf{t}})/\sigma_u^2$ is obtained from the corresponding matrix in the unblocked design.

For unstructured treatments, we might consider the efficiency factors for all possible pairwise comparisons of treatments, $t_s - t_r$.

Unstructured treatments

We will obtain an efficient design for the introductory example.

We can have 4 replicates of each treatment.

There are ${}^6C_2 = 15$ comparisons of interest.

$6 \times^4 C_2 = 36$ comparisons can be made within blocks.

Each pair of treatments should appear together in blocks at least twice, 6 pairs a third time: 12 23 34 45 56 16.

Unstructured treatments

Block					
I	II	III	IV	V	VI
1	1	1	1	2	3
2	2	2	4	3	4
3	3	5	5	4	5
4	6	6	6	5	6

Efficiency factors:

$$\hat{t}_2 - \hat{t}_1 : 93.3\%;$$

$$\hat{t}_3 - \hat{t}_1 : 87.0\%;$$

$$\hat{t}_4 - \hat{t}_1 : 86.7\%.$$

The blocked design is clearly better if

$$\frac{\sigma_u^2}{\sigma^2} > \frac{1}{0.867} = 1.153.$$

Unstructured treatments

For small problems, it is easy to obtain a good design by hand. For larger problems we require a computer search.

I assume that the user will input the treatment design and the block structure and the program will search of the optimal arrangement of treatments to blocks.

Other methods search simultaneously for the optimal treatment design and its optimal arrangement in blocks. This implies a fixed blocks view, i.e. inter-block information is lost. In the randomization view, the information is all there, but is split between the strata.

To be able to find a design in any situation a program needs to use:

- a criterion for deciding which design is best; and
- an algorithm for searching many possible designs.

Unstructured treatments

The first computational approach that should be considered is a complete search. This might be feasible if there is a small number of large blocks, but otherwise is likely to be computationally prohibitive.

Most blocking algorithms are based on interchange algorithms:

1. Start with a random assignment of treatments to blocks;
2. Systematically interchange pairs of treatments between blocks, keeping any interchanges which improve the design;

Usually we do this several (100?) times.

Efficiency criteria for blocking

The choice of criterion for blocking is less obvious than for choosing a treatment design.

Consider arranging in blocks a treatment design which is much better for estimating some treatment comparisons than others, e.g. a design which is good for estimating main effects, but which estimates interactions imprecisely.

Do we want the blocked design to preserve the features of the treatment design or to compensate for the weaknesses of the treatment design?

Many reasonable criteria use the efficiency factors for the relevant treatment comparisons or parameters, rather than the variances.

Efficiency criteria for blocking

Partition $\mathbf{X}$ as $[\mathbf{1}\ \mathbf{X}_1\ \mathbf{X}_2]$, where $\mathbf{X}_1$ corresponds to block effects and $\mathbf{X}_2$ to treatment parameters, and let $\mathbf{R}$ be a diagonal matrix with elements $\sqrt{r_i}$, where r_i is the replication of treatment i. Then a scaled information matrix for treatments is given by

$$\mathbf{A} = \mathbf{I} - \mathbf{R}^{-1}\mathbf{X}_2'\mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2\mathbf{R}^{-1}.$$

The *canonical efficiency factors* are the eigenvalues of $\mathbf{A}$ and therefore easy to compute. The corresponding contrasts are called the *basic contrasts*.

In general the basic contrasts do not represent the contrasts of interest, but in some cases they do.

Efficiency criteria for blocking

For unstructured treatments, it is often assumed that we are equally interested in all pairwise treatment comparisons, $t_s - t_r$.

For equally replicated treatments it can be shown that:

- The harmonic mean of the canonical efficiency factors is proportional to the harmonic mean of the efficiency factors for pairwise comparisons. In this specific context, this particular L-efficiency criterion is usually called A-efficiency.
- The smallest canonical efficiency factor is proportional to the smallest efficiency factor for any contrast and thus represents E-efficiency.
- The geometric mean of the efficiency factors is proportional to D-efficiency.

Other blocking criteria often defined with respect to the canonical efficiency factors are:

- M-efficiency is the (arithmetic) mean of the canonical efficiency factors.
- S-efficiency is the mean of the squared canonical efficiency factors.
- (M,S)-efficiency orders designs first by M-efficiency and then by S-efficiency.

Blocking factorial designs

Example
An experiment was to be conducted on a food extrusion process used for mixing pastry dough. The objective was to see how the initial moisture content, feed flow rate and screw speed affected various properties of the pastry - size and shape, strength and colour - with a view to developing a control system. Only four runs could be carried out in one day and day to day differences were expected. It was decided to do a three level central composite design with two replicates of each of the factorial points, one set of axial points and six centre points. How should this design be arranged in blocks?

Blocking factorial designs

Because factorial structures often lead to a large number of treatments, incomplete blocks will often be necessary. Up to now we have allocated treatments to blocks assuming all comparisons are of equal importance. With factorial treatments, this is not the case: we are primarily interested in main effects, secondarily in two-factor interactions, and so on.

If the factors are continuous, we are primarily concerned with linear effects, secondarily with quadratic and linear$\times$linear effects, and so on.

Qualitative Factors

Within each block we aim to get:

- each level of each factor appearing (as near as possible) equally often;
- each combination of levels for each pair of factors appearing (as near as possible) equally often;
- each combination of levels for each set of three factors appearing (as near as possible) equally often;
- and so on.

Over all blocks we aim to get each pair of combinations of all factors appearing together (as near as possible) equally often.

Example

Arrange a 2^3 factorial in 2 blocks of 4.

Block I			Block II		
A	B	C	A	B	C
0	0	0	0	0	1
0	1	1	0	1	0
1	0	1	1	0	0
1	1	0	1	1	1

Note that the two blocks contain the half replicates with defining contrasts $I \equiv ABC$ and $I \equiv -ABC$.

Therefore, we can estimate all main effects and two-factor interactions, but not the three factor interaction. We say ABC is *confounded* with the block effect.

Interblock Information

When arranging factorial treatments in blocks we ensure that the important contrasts (factorial effects) can be estimated at the within-block level.

The less important effects can then be estimated at the inter-block level.

This will usually give very little information about *these* effects and so does not have any impact on how we should design experiments beyond possibly restricting randomization of treatment groups to blocks.

Example

Four replicates of the 2^3 design in blocks of 4.

By arranging each replicate in a superblock we get the following analysis of variance:

Source of Variation	df
Superblock error	3
Superblock total	3
ABC	1
Block error	3
Block total	7
A	1
B	1
C	1
AB	1
AC	1
BC	1
Error	18
Total	31

Criteria for blocking factorial designs

Lists of regular designs, like the one above, are available, as are packages for constructing them.

More generally, we will use a complete search, or an interchange algorithm.

The appropriate blocking criteria can be the same as for choice of treatments, e.g. weighted-A-efficiency, D-efficiency, etc.

Given a set of comparisons of interest, it might be sensible to give them equal weight in an L-efficiency criterion. This is equivalent to minimizing the harmonic mean of the efficiency factors of the comparisons of interest. This is occasionally referred to as A-efficiency.

Criteria for blocking factorial designs

Minimizing the harmonic mean of the efficiency factors of the *parameters* is sometimes referred to as A-efficiency.

Finally, minimizing the harmonic mean of the subset of the parameters of interest (i.e. treatment comparisons) is sometimes referred to as A-efficiency, or A_s-efficiency. Only this makes sense.

Continuing the analogy, for general contrasts of interest, define weighted-M-efficiency to be a weighted mean of the efficiency factors of the contrasts or parameters of interest (referred to as the "weighted mean efficiency factor"). Weighted-S-efficiency and weighted-(M,S)-efficiency could be defined in a similar way.