Experimental Design

Unit 5

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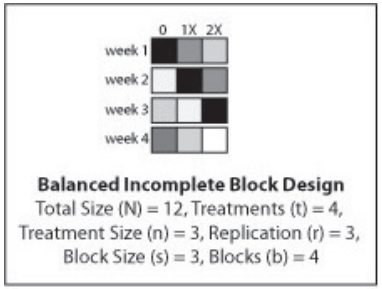
7.1 Introduction to Balanced incomplete block designs (BIBD)

The CBD and LSD introduced in Chapters 4 and 5 share special structure that leads to simple and desirable characteristics in data analysis. In particular, they are orthogonally blocked designs, composed of blocks of the smallest size (t units) for which this is possible.



Sometimes it is not possible or not reasonable to assign each treatment to each block. This results in incomplete blocks, that is, blocks in which only a subset of treatments are assigned.

The total number of units and observations n now is $b \cdot k$ rather than $b \cdot t$, i.e. now the block size, or number of units in each block is k which is less than t as in CBDs.

Balanced incomplete block designs (BIBD) (cont.)

Balanced Incomplete Block Designs (BIBDs) are a special class of designs which, as their name suggests, maintain statistically desirable „balance“ properties.

An incomplete block design is *balanced* when three requirements are met

- Each treatment is applied to at most one unit in each block.
- Each treatment is applied to a unit in the same number of blocks (*first-order balance*). The common number of units per treatment then is $r = \frac{b\,k}{t}$
- Each pair of treatments is applied to two units in the same number of blocks (*second-order balance*). The common number of blocks in which each pair of treatments appear is $\pi = \frac{r(k-1)}{t-1}$.

7.1.2 Existence and construction of BIBDs

There are many combinations of values of t, k, and b for which a BIBD does not exist. A necessary, but not sufficient, condition for the existence of a BIBD is:

For given t, k, and b, a BIBD cannot exist unless:

- $r = \frac{b\,k}{t}$ is an integer, and
- $\pi = \frac{r(k-1)}{t-1} = \frac{b\,k(k-1)}{t(t-1)}$ is an integer.

Example: $t = 7$, $k = 5$, $b = 21$.

Easiest construction: each block contains one of the $\binom{t}{k}$ subset (may not be the smallest design!).

Any BIBD in b blocks can be expanded to a BIBD in $m \cdot b$ blocks, $2 \leq m \in \mathbb{N}$, by including m „copies“ of each required block. The values of r and π for the (larger) BIBD are each also increased by a factor of m.

7.2 A model

The form of an effects model for a BIBD is the same as that for a CBD:

$$y_{ij} = \alpha + \beta_i + \tau_j + \varepsilon_{ij} \qquad i = 1, \ldots, b \quad j \in S(i)$$

$$\varepsilon_{ij} \text{ iid with } \quad \mathsf{E}(\varepsilon_{ij}) = 0 \quad \text{and} \quad \mathsf{Var}(\varepsilon_{ij}) = \sigma^2$$

where $S(i)$ is the set of k treatments assigned to experimental units in block i.

The model degrees of freedom is $\mathsf{df} = b + t - 1$ like in the CBD, because all treatment effects have to be estimated although not all treatments appear in each block.

7.2.1 Graphical logic

Using „block-corrected“ observations for boxplots is not so reasonable with BIBDs since each block (and so each block average) represents only a subset of treatments. The correction in BIBDs concerns a different subset of treatments in each block, and so the recipe for CBD does not produce the desired result.

If t is small we may construct a boxplot of differences for each pair of treatments, using only data from the π blocks in which both treatments have been applied to units:

$$d_{ijj'} = y_{ij} - y_{ij'} \qquad j \in S(i) \quad \text{and} \quad j' \in S(i),\ j \neq j'$$

Each $d_{ijj'}$ has mean $\tau_j - \tau_{j'}$ and variance $2\sigma^2$, and so reflects only relative characteristics of treatments j and j'.

7.3 Matrix formulation

A matrix representation follows the general form of that for a CBD:

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta} + \mathbf{X}_2\boldsymbol{\tau} + \boldsymbol{\varepsilon} \qquad \boldsymbol{\varepsilon} \sim \mathbf{N}(\mathbf{0}; \sigma^2\mathbf{I})$$

- $\boldsymbol{\beta}$ is the $(b+1)$-vector of nuisance parameters $\alpha, \beta_1, \ldots, \beta_b$
- $\boldsymbol{\tau}$ is the t-vector of treatment parameters
- $\mathbf{y}$ and $\boldsymbol{\varepsilon}$ are n-vectors of responses and random errors where $n = b \cdot k$
- $\mathbf{X}_1$ takes the form that would be used in a CBD with k rather than t treatments:

$$\mathbf{X}_1 = \begin{pmatrix} \mathbf{1}_k & \mathbf{1}_k & \mathbf{0}_k & \cdots & \mathbf{0}_k \\ \mathbf{1}_k & \mathbf{0}_k & \mathbf{1}_k & \cdots & \mathbf{0}_k \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{1}_k & \mathbf{0}_k & \mathbf{0}_k & \cdots & \mathbf{1}_k \end{pmatrix}$$

- $\mathbf{H}_1$ also takes the same form as it would in a CBD with blocks of size k.

Matrix formulation (cont.)

$\mathbf{X}_2$ is more difficult to write simply, but can be characterized by noting

- each row consists of zeros with the exception of a single 1,
- the total of elements in any column of $\mathbf{X}_2$ is r,
- the inner product of any two columns of $\mathbf{X}_2$ is zero, i.e. the columns of $\mathbf{X}_2$ are orthogonal
- the group of rows numbered $((i-1)k+1, (i-1)k+2, \ldots, ik)\,,\ i = 1, \ldots, b$, i.e. the rows of the i-th block, contain ones placed according to each element of $S(i)$.

In the general case, a given row of $\mathbf{X}_{2|1}$ contains three unique values:

- $1 - \frac{1}{k}$ in the column corresponding to the treatment applied to this unit
- $-\frac{1}{k}$ in columns corresponding to the $k-1$ other treatments applied to units in this block
- 0 in columns corresponding to treatments not applied to any unit in this block.

Matrix formulation (cont.)

Just as in the case of the CBD contrasts are the only estimable linear combinations of the elements of $\boldsymbol{\tau}$ and we may estimate any such contrast. For the information matrix $\mathcal{I} = \mathbf{X}_{2|1}^T \mathbf{X}_{2|1}$ we have to examine the j-th column of $\mathbf{X}_{2|1}$ (corresponding to treatment j), it contains:

- r elements of value $1 - \frac{1}{k}$, corresponding to the r experimental runs in which treatment j is applied
- $r(k-1)$ elements of value $-\frac{1}{k}$ corresponding to runs in which other treatments were applied, but which are grouped in blocks where treatment j was also applied
- $k(b-r)$ elements of value zero corresponding to runs in blocks where treatment j was not applied.

The sum of squared elements in any column of $\mathbf{X}_{2|1}$ is $\frac{r(k-1)}{k} = \frac{\pi(t-1)}{k}$, this is the common diagonal element of $\mathcal{I}$.

Matrix formulation (cont.)

The inner product of any pair of distinct columns of $\mathbf{X}_{2|1}$ is comprised of:

- 2π terms of value $-(1-\frac{1}{k})\frac{1}{k}$ corresponding to runs receiving one of the two treatments, from blocks in which they are both applied
- $\pi(k-2)$ terms of value $\frac{1}{k^2}$ corresponding to runs receiving neither of the two treatments, from blocks in which they are both applied (to other units)
- $(b-\pi)k$ terms of value 0 corresponding to runs from blocks in which at least one of the two treatments is not applied.

So the inner product for two such columns of $\mathbf{X}_{2|1}$ is $-\frac{\pi}{k}$, this is the common off-diagonal element of $\mathcal{I}$.

All together the information matrix $\mathcal{I}$ is

$$\mathcal{I} = \frac{\pi\, t}{k}\left(\mathbf{I} - \frac{1}{t}\mathbf{J}\right)$$

Matrix formulation (cont.)

Using the above information the system of reduced normal equations $\mathcal{I}\hat{\boldsymbol{\tau}} = \mathbf{X}_{2|1}^T\mathbf{y}$ can be written as

$$\frac{\pi\, t}{k}\left(\mathbf{I} - \frac{1}{t}\,\mathbf{J}\right)\hat{\boldsymbol{\tau}} = \mathbf{T} - \frac{1}{k}\,\mathbf{X}_2^T\mathbf{X}_1\mathbf{B} = \mathcal{Q}$$

where $\mathbf{T}$ is the t-vector of treatment totals and $\mathbf{B}$ is the b-vector of block totals.

The elements of $\mathcal{Q}$ are also called „adjusted treatment totals“.

Matrix formulation (cont.)

This leads to the form of the estimate for any contrast in the treatment parameters:

$$\widehat{\mathbf{c}^T\boldsymbol{\tau}} = \frac{k}{\pi\, t}\,\mathbf{c}^T\mathcal{Q}$$

The form of the estimate for unblocked or orthogonally blocked experiments with r units assigned to each treatment looks similar:

$$\widehat{\mathbf{c}^T\boldsymbol{\tau}} = \frac{1}{r}\,\mathbf{c}^T\mathbf{T}$$

but $\mathbf{T}$ and $\mathcal{Q}$ are not equal and $r \neq \frac{\pi\, t}{k}$, reflecting the fact that treatments and blocks are not orthogonal in a BIBD.

Matrix formulation (cont.)

Because of the nonorthogonality of blocks and treatments the variance decomposition is different from CBD. The decomposition for CBD with r blocks is

$$\mathsf{TSS} = \mathsf{SST} + \mathsf{SSB} + \mathsf{SSE}$$

where SSB and SST are the sum of squares associated with the blocks and treatments respectively.

$$\mathsf{SST} = \sum_{j=1}^{t} r(\bar{y}_j - \bar{y})^2 \qquad \mathsf{SSB} = \sum_{i=1}^{r} t(\bar{y}_i - \bar{y})^2 \qquad \mathsf{TSS} = \sum_{i,j} (y_{ij} - \bar{y})^2$$

Matrix formulation (cont.)

Because of the nonorthogonality of blocks and treatments in a BIBD some of the variation in the data can be attributed to either blocks or treatments.

If we assigns all of this variation to blocks SSB is computed as above, and SST (which now quantifies variation associated for treatments after „adjustment“ for blocks) can be written for a BIBD as

$$\mathsf{SST}_{BIBD} = \sum_j \frac{k}{\pi\, t} Q_j^2$$

SSE can be computed as $\mathsf{SSE} = \mathsf{TSS} - \mathsf{SSB} - \mathsf{SST}_{BIBD}$.

This residual sum of square differs from the SSE from a CBD.

7.4. Influence of design on quality of inference

WE compare to CRDs of the same size.

The ratio of estimation variances is thus

$$\frac{\mathsf{Var}_{BIBD}}{\mathsf{Var}_{CRD}} = \frac{kr\sigma^2_{\mathsf{BIBD}}}{\pi t\sigma^2_{\mathsf{CRD}}} = \frac{k(t-1)}{t(k-1)}\frac{\sigma^2_{\mathsf{BIBD}}}{\sigma^2_{\mathsf{CRD}}}$$

Same holds for the comparison to CBDs, but here the reduction cannot come from the reduction in variance due to blocking.

7.5 More general constructions

7.5.1 Extended complete block designs

These designs are similar to the augmented CBD, in that the number of units in each block is larger than the number of treatments. In extended complete block designs, each treatment is assigned to one of the first t units in each block, and a BIBD is used to determine the treatment assignments for the „extra“ units.

We have b blocks of $k > t$ units each and t treatments, and b, k, and t are such that a BIBD exists for t treatments in b blocks of size $k' = k - t$ (extra units) with design parameters $r' = \frac{b\,k'}{t}$ and $\pi' = \frac{r'(k'-1)}{t-1}$.

So k' treatments are applied to *two* randomly selected units in each block and the remaining $t - k'$ are applied to just *one* unit in the block.

The result is a design that has first- and second-order balance among treatments and that affords $b\,k'$ „pure error“ degrees of freedom in the within-block replications for the estimation of σ^2.

7.5.2 Partially balanced incomplete block designs

A *partially balanced incomplete block design* (PBIBD), like a BIBD, is a design for comparing t treatments in b blocks of $k < t$ units each, that requires each treatment to be applied to one unit in each of r blocks - the same first-order balance property required of BIBDs.

However, the „partial“ second-order balance requirements of a PBIBD are less stringent.

- For each treatment i, the remaining $t - 1$ treatments may be divided into two groups; call these A_i and B_i. The treatments identified in A_i are called *first associates* of treatment i, and those identified in B_i are called *second associates* of treatment i.
- Any two treatments that are first associates appear together in $\pi_1 > \pi'$ blocks. Any two treatments that are second associates appear together in π_2 blocks.
- For any treatment i, A_i contains t_1 elements, and B_i contains t_2 elements, $t_1 + t_2 = t - 1$.

Partially balanced incomplete block designs (cont.)

- For any two treatments that are first associates, say treatments i and j,
  - A_i and A_j have p_{11} elements in common,
  - A_i and B_j (or A_j and B_i) have p_{12} elements in common, and
  - B_i and B_j have p_{22} elements in common.
- For any two treatments that are second associates, say treatments i and j,
  - A_i and A_j have q_{11} elements in common,
  - A_i and B_j (or A_j and B_i) have q_{12} elements in common, and
  - B_i and B_j have q_{22} elements in common.

Hence, the inter-related design parameters (values specifying the structure and properties of the design) are t, b, k, t_1, t_2, π_1, π_2, p_{11}, p_{12}, p_{22}, q_{11}, q_{12}, and q_{22}. Extensive tables of PBIBD designs have been published (Clatworthy, 1973).

Examples

Here comes a BIBD
for $t = 5$ treatments
in $b = 10$ blocks
of size $k = 3$

1	1	1	1	1	1	2	2	2	3
2	2	2	3	3	4	3	3	4	4
3	4	5	4	5	5	4	5	5	5

Each treatment is applied to a unit in $r = \frac{b\,k}{t} = \frac{10 \cdot 3}{5} = 6$ blocks and
Each pair of treatments is applied to two units in $\pi' = \frac{r(k-1)}{t-1} = \frac{6(3-1)}{5-1} = 3$ blocks.

This design with the same
b, t, k and r is no BIBD

1	3	5	2	4	1	3	5	2	4
2	4	1	3	5	2	4	1	3	5
3	5	2	4	1	3	5	2	4	1

Treatments 1 and 2 are applied in the same block 4 times but treatments 1 and 3 are applied in the same block just 2 times. So there is no common value of π' and no second-order balance. But the design has first-order balance and is a PBIBD.

Partially balanced incomplete block designs (cont.)

Each pair of treatments is applied together in blocks with frequencies:

treatments	(1,2)	(1,3)	(1,4)	(1,5)	(2,3)	(2,4)	(2,5)	(3,4)	(3,5)	(4,5)
frequencies	4	2	2	4	4	2	2	4	2	4

The first and second associates for each treatment are

treatments	1	2	3	4	5
1^{st} associates	{2,5}	{1,3}	{2,4}	{3,5}	{1,4}
2^{nd} associates	{3,4}	{4,5}	{1,5}	{1,2}	{2,3}

with $\pi_1 = 4$, and $\pi_2 = 2$. There are two associate classes for each treatment, so these designs are also designated PBIBD(2).

The more general class of designs also includes subclasses PBIBD(m) with $m = 3, 4, \ldots, t-1$ for more associate classes.