Laplacian eigenvalues and optimality: I. Block designs

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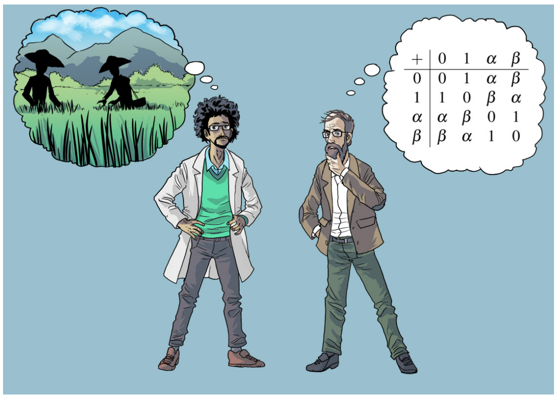
Mathematicians and statisticians

There is a very famous joke about Bose's work in Giridh. Professor Mahalanobis wanted Bose to visit the paddy fields and advise him on sampling problems for the estimation of yield of paddy. Bose did not very much like the idea, and he used to spend most of the time at home working on combinatorial problems using Galois fields. The workers of the ISI used to make a joke about this. Whenever Professor Mahalanobis asked about Bose, his secretary would say that Bose is working in fields, which kept the Professor happy.

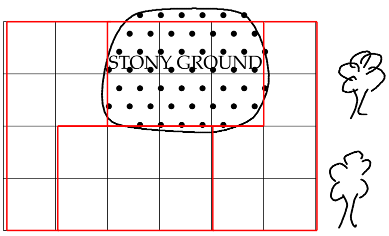
Bose memorial session, in *Sankhyā* **54** (1992)
(special issue devoted to the memory of Raj Chandra Bose),
i–viii.

Mathematicians and statisticians



An experiment in a field

We have 6 varieties of cabbage to compare in this field.
How do we avoid bias?



Partition the experimental units into homogeneous blocks and plant each variety on one plot in each block.

An experiment on people

Several studies have suggested that drinking red wine gives some protection against heart disease, but it is not known whether the effect is caused by the alcohol or by some other ingredient of red wine. To investigate this, medical scientists enrolled 40 volunteers into a trial lasting 28 days. For the first 14 days, half the volunteers drank two glasses of red wine per day, while the other half had two standard drinks of gin. For the remaining 14 days the drinks were reversed: those who had been drinking red wine changed to gin, while those who had been drinking gin changed to red wine. On days 14 and 28, the scientists took a blood sample from each volunteer and measured the amount of inflammatory substance in the blood.

Each experimental unit consist of one volunteer for 14 days.
So there are 80 experimental units.
Each volunteer forms a block of size 2.

The treatments are the 2 types of drink.

An experiment on diffusion of proteins

A post-doc added from 0 to 4 extra green fluorescent proteins to cells of *Escherichia coli*, adding 0 to 10 cells, 1 to 10 further cells, and so on. Then she measured the rate of diffusion of proteins in each of the 50 cells.

This is what she did.

Monday	Tuesday	Wednesday	Thursday	Friday
0000000000	1111111111	2222222222	3333333333	4444444444

Are the perceived differences caused by differences in size?

Did she get better at preparing the samples as the week wore on?

Were there environmental changes in the lab that could have contributed to the differences?

Diffusion of proteins: continued

What she did.

Monday	Tuesday	Wednesday	Thursday	Friday
0000000000	1111111111	2222222222	3333333333	4444444444

Better to regard each day as a block.

Monday	Tuesday	Wednesday	Thursday	Friday
0011223344	0011223344	0011223344	0011223344	0011223344

There may still be systematic differences within each day,
so better still, randomize within each day.

Monday	Tuesday	Wednesday	Thursday	Friday
1040223134	2230110443	1421324030	4420013312	3204320411

An experiment on detergents

In a consumer experiment, twelve housewives volunteer to test new detergents. There are 16 new detergents to compare, but it is not realistic to ask any one volunteer to compare this many detergents.
Each housewife tests one detergent per washload for each of four washloads, and assesses the cleanliness of each washload.

The experimental units are the washloads.
The housewives form 12 blocks of size 4.

The treatments are the 16 new detergents.

Experiments in blocks

I have v treatments that I want to compare.
I have b blocks, with k plots in each block.

blocks	b	k	treatments	v
contiguous plots	4	6	cabbage varieties	6
volunteers	40	2	drinks	2
days	5	10	numbers of cells	5
housewives	12	4	detergents	16

How should I choose a block design?
How should I randomize it?
How should I analyse the data after the experiment?
What makes a block design good?

Complete block designs: construction and randomization

For a complete-block design,
there are v treatments, and b blocks of size v.

Construction Each treatment occurs on one plot per block.
Randomization Within each block independently,
randomize the order of the treatments.

Statistical Model

Let $f(\omega)$ = treatment on plot ω
$g(\omega)$ = block containing plot ω.

We assume that the response Y_ω on plot ω satisfies:

$$Y_\omega = \tau_{f(\omega)} + \beta_{g(\omega)} + \varepsilon_\omega,$$

where τ_i is a constant depending on treatment i,
β_j is a constant depending on block j,

and the ε_ω are independent (normal) random variables with zero mean and variance σ^2.

We can replace τ_i and β_j by $\tau_i + c$ and $\beta_j - c$ without changing the model. So we cannot estimate $\tau_1, \ldots, \tau_v$.

But we can estimate treatment differences $\tau_i - \tau_l$,
and we can estimate sums $\tau_i + \beta_j$.

Estimating treatment differences

$$Y_\omega = \tau_{f(\omega)} + \beta_{g(\omega)} + \varepsilon_\omega$$

An estimator for $\tau_1 - \tau_2$ is

- best if it has minimum variance subject to the other conditions;
- linear if it is a linear combination of $Y_1, Y_2, \ldots, Y_{bk}$;
- unbiased if its expectation is equal to $\tau_1 - \tau_2$.

The best linear unbiased estimator of $\tau_1 - \tau_2$ is

(average response on treatment 1) − (average response on treatment 2).

The variance of this estimator is

$$\frac{2\sigma^2}{bk/v} = \frac{2\sigma^2}{b}.$$

Residuals

The best linear unbiased estimator of $\tau_i + \beta_j$ is

(average response on treatment i) + (average response on block j)
−(average response overall).

Write this $\hat{\tau}_i + \hat{\beta}_j$.

The residual on experimental unit ω is

$$Y_\omega - \hat{\tau}_{f(\omega)} - \hat{\beta}_{g(\omega)}.$$

The residual sum of squares RSS $= \sum_\omega (Y_\omega - \hat{\tau}_{f(\omega)} - \hat{\beta}_{g(\omega)})^2 =$

$$\sum_\omega Y_\omega^2 - \sum_{i=1}^{v} \frac{(\text{total on treatment } i)^2}{bk/v} - \sum_{j=1}^{b} \frac{(\text{total on block } j)^2}{k} + \frac{(\sum_\omega Y_\omega)^2}{bk}.$$

Estimating variance

Theorem
$\mathbb{E}(\text{RSS}) = (bk - b - v + 1)\sigma^2$.

Hence
$$\frac{\text{RSS}}{(bk - b + v - 1)}$$
is an unbiased estimator of σ^2.

Comments

1. We are not usually interested in the block parameters β_j.
2. If $k = vs$ and each treatment occurs s times in each block, then estimation is similar.
   The formulas in the preceding three slides involve k as well as v; and they should be correct in this more general case.

Incomplete-block designs

For an incomplete-block design,
there are v treatments, and b blocks of size k, where $2 \leq k < v$.

Construction How do we choose a suitable design?

Randomization
- Randomize the order of the blocks, because they do not all have the same treatments.
- Within each block independently, randomize the order of the treatments.

Two designs with $v = 15$, $b = 7$, $k = 3$: which is better?

Conventions: columns are blocks;
order of treatments within each block is irrelevant;
order of blocks is irrelevant.

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

replications differ by ≤ 1

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

queen-bee design

The replication of a treatment is its number of occurrences.

A design is a queen-bee design if there is a treatment that occurs in every block.

Average replication $= \bar{r} = bk/v = 1.4$.

Equireplicate designs

Theorem
If every treatment is replicated r times then $vr = bk$.

Proof.
Count the number of experimental units in two different ways. □

Two designs with $v = 5$, $b = 7$, $k = 3$: which is better?

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

binary

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

non-binary

A design is binary if no treatment occurs more than once in any block.

We shall not consider any design in which there is any block having the same treatment on every plot.

Average replication $= \bar{r} = bk/v = 4.2$.

Two designs with $v = 7$, $b = 7$, $k = 3$: which is better?

1	2	3	4	5	6	7
2	3	4	5	6	7	1
4	5	6	7	1	2	3

balanced (2-design)

1	2	3	4	5	6	7
2	3	4	5	6	7	1
3	4	5	6	7	1	2

non-balanced

A binary design is balanced if every pair of distinct treatments occurs together in the same number of blocks.
(These are also called 2-designs.)

Average replication $=$ every replication $= \bar{r} = bk/v = 3$.

Balanced incomplete-block designs

Theorem
If a binary design is balanced, with every pair of distinct treatments occuring together in λ blocks, then the design is equi-replicate and $r(k-1) = \lambda(v-1)$.

Proof.
Suppose that treatment i has replication r_i, for $i = 1, \ldots, v$. The design is binary, so treatment i occurs in r_i blocks. Each of these blocks has $k-1$ other experimental units, each with a treatment other than i. Each other treatment must occur on λ of these experimental units. There are $v-1$ other treatments, and so

$$r_i(k-1) = \lambda(v-1).$$

In particular, $r_i = r = \lambda(v-1)/(k-1)$ for $i = 1, \ldots, v$. $\square$

Statistical Model

$$\begin{aligned} f(\omega) &= \text{treatment on plot } \omega \\ g(\omega) &= \text{block containing plot } \omega. \end{aligned}$$

We assume that the response Y_ω on plot ω satisfies:

$$Y_\omega = \tau_{f(\omega)} + \beta_{g(\omega)} + \varepsilon_\omega,$$

where τ_i is a constant depending on treatment i,
β_j is a constant depending on block j.

Rewritten in vector form:

$$Y = X\tau + Z\beta + \varepsilon,$$

$$\text{where} \quad X_{\omega,i} = \begin{cases} 1 & \text{if } f(\omega) = i \\ 0 & \text{otherwise,} \end{cases}$$

$$\text{and} \quad Z_{\omega,j} = \begin{cases} 1 & \text{if } g(\omega) = j \\ 0 & \text{otherwise.} \end{cases}$$

Small example: $v = 8$, $b = 4$, $k = 3$

B1	B2	B3	B4
1	2	3	4
2	3	4	1
5	6	7	8

$$X = \begin{array}{c} \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \end{array} \qquad Z = \begin{array}{c} \begin{matrix} \text{B1} & \text{B2} & \text{B3} & \text{B4} \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

The ‘same block’ indicator matrix B

$$ZZ^\top = B,$$

$$\text{where} \quad B_{\alpha,\omega} = \begin{cases} 1 & \text{if } \alpha \text{ and } \omega \text{ are in the same block} \\ 0 & \text{otherwise.} \end{cases}$$

Small example continued

B1	B2	B3	B4
1	2	3	4
2	3	4	1
5	6	7	8

$$Z = \begin{array}{c} \begin{matrix} \text{B1} & \text{B2} & \text{B3} & \text{B4} \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array} \qquad B = ZZ^\top = \begin{bmatrix} 1&1&1&0&0&0&0&0&0&0&0&0 \\ 1&1&1&0&0&0&0&0&0&0&0&0 \\ 1&1&1&0&0&0&0&0&0&0&0&0 \\ 0&0&0&1&1&1&0&0&0&0&0&0 \\ 0&0&0&1&1&1&0&0&0&0&0&0 \\ 0&0&0&1&1&1&0&0&0&0&0&0 \\ 0&0&0&0&0&0&1&1&1&0&0&0 \\ 0&0&0&0&0&0&1&1&1&0&0&0 \\ 0&0&0&0&0&0&1&1&1&0&0&0 \\ 0&0&0&0&0&0&0&0&0&1&1&1 \\ 0&0&0&0&0&0&0&0&0&1&1&1 \\ 0&0&0&0&0&0&0&0&0&1&1&1 \end{bmatrix}$$

More matrices

matrix	X	Z	B	R	N	Λ	L	C
dimensions	$bk \times v$	$bk \times b$	$bk \times bk$	$v \times v$	$v \times b$	$v \times v$	$v \times v$	$v \times v$

$$X_{\omega,i} = \begin{cases} 1 & \text{if } f(\omega) = i \\ 0 & \text{otherwise,} \end{cases} \qquad Z_{\omega,j} = \begin{cases} 1 & \text{if } g(\omega) = j \\ 0 & \text{otherwise.} \end{cases}$$

$$ZZ^\top = B \qquad Z^\top Z = kI_b$$

$X^\top X = R =$ diagonal matrix of treatment replications

$X^\top Z = N =$ incidence matrix

$N_{ij} =$ number of times that treatment i occurs in block j.

$NN^\top = \Lambda =$ concurrence matrix

λ_{ij} = number of occurrences of i and j in the same block
= concurrence of treatments i and j

$L = kR - \Lambda =$ Laplacian matrix $\qquad C = \frac{1}{k}L =$ information matrix

Small example continued again

B1	B2	B3	B4
1	2	3	4
2	3	4	1
5	6	7	8

$$Z^\top Z = 3I_4$$

$$X^\top X = R = \begin{array}{cc} & \begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{array} \\ \begin{array}{c} 1\\2\\3\\4\\5\\6\\7\\8 \end{array} & \begin{bmatrix} 2&0&0&0&0&0&0&0\\ 0&2&0&0&0&0&0&0\\ 0&0&2&0&0&0&0&0\\ 0&0&0&2&0&0&0&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&1&0\\ 0&0&0&0&0&0&0&1 \end{bmatrix} \end{array}$$

Small example: incidence matrix

B1	B2	B3	B4
1	2	3	4
2	3	4	1
5	6	7	8

$$N = X^\top Z = \begin{array}{cc} & \begin{array}{cccc} B1 & B2 & B3 & B4 \end{array} \\ \begin{array}{c} 1\\2\\3\\4\\5\\6\\7\\8 \end{array} & \begin{bmatrix} 1&0&0&1\\ 1&1&0&0\\ 0&1&1&0\\ 0&0&1&1\\ 1&0&0&0\\ 0&1&0&0\\ 0&0&1&0\\ 0&0&0&1 \end{bmatrix} \end{array}$$

Small example: concurrence matrix

B1	B2	B3	B4
1	2	3	4
2	3	4	1
5	6	7	8

$$\Lambda = NN^\top = \begin{array}{cc} & \begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{array} \\ \begin{array}{c} 1\\2\\3\\4\\5\\6\\7\\8 \end{array} & \begin{bmatrix} 2&1&0&1&1&0&0&1\\ 1&2&1&0&1&1&0&0\\ 0&1&2&1&0&1&1&0\\ 1&0&1&2&0&0&1&1\\ 1&1&0&0&1&0&0&0\\ 0&1&1&0&0&1&0&0\\ 0&0&1&1&0&0&1&0\\ 1&0&0&1&0&0&0&1 \end{bmatrix} \end{array}$$

Small example: Laplacian matrix

B1	B2	B3	B4
1	2	3	4
2	3	4	1
5	6	7	8

$$L = kR - \Lambda = \begin{array}{cc} & \begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{array} \\ \begin{array}{c} 1\\2\\3\\4\\5\\6\\7\\8 \end{array} & \begin{bmatrix} 4&-1&0&-1&-1&0&0&-1\\ -1&4&-1&0&-1&-1&0&0\\ 0&-1&4&-1&0&-1&-1&0\\ -1&0&-1&4&0&0&-1&-1\\ -1&-1&0&0&2&0&0&0\\ 0&-1&-1&0&0&2&0&0\\ 0&0&-1&-1&0&0&2&0\\ -1&0&0&-1&0&0&0&2 \end{bmatrix} \end{array}$$

Concurrence

$$\lambda_{ij} = \sum_{m=1}^{b} N_{im}N_{jm}$$

= the number of ordered pairs of experimental units (α, ω) with $g(\alpha) = g(\omega)$ (same block) and $f(\alpha) = i$ and $f(\omega) = j$.

If the design is binary, then $\lambda_{ii} = r_i$ for $i = 1, \ldots, v$.

Counting pairs (α, ω) with $g(\alpha) = g(\omega)$ and $f(\alpha) = i$ shows that

$$r_i k = \sum_{j=1}^{v} \lambda_{ij} = \lambda_{ii} + \sum_{j \neq i} \lambda_{ij}.$$

$$L_{ii} = r_i k - \lambda_{ii} = \sum_{j \neq i} \lambda_{ij}$$

If $j \neq i$ then $L_{ij} = -\lambda_{ij}$.

Theorem

The entries in each row of the Laplacian matrix sum to zero.

Fisher's Inequality

Theorem
If the design is balanced, then $b \geq v$.

Proof.
The design is binary, so

$$\Lambda = rI_v + \lambda(J_v - I_v) = (r-\lambda)\left(I_v - \frac{J_v}{v}\right) + [\lambda(v-1)+r]\frac{J_v}{v},$$

where I_v is the $v \times v$ identity matrix and J_v is the $v \times v$ all-1 matrix. The eigenvalues of Λ are $r - \lambda$ and $\lambda(v-1)+r$.
But $r(k-1) = \lambda(v-1)$ and $k < v$ so $\lambda < r$, so $r - \lambda > 0$ and $\lambda(v-1) + r = rk > 0$, so these eigenvalues are non-zero. Hence

$$v = \operatorname{rank}(\Lambda) = \operatorname{rank}(NN^\top) = \operatorname{rank}(N^\top N) \leq b.$$

$\square$

Laplacian matrices for two designs with $v = 5$, $b = 7$, $k = 3$

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

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

$$\begin{bmatrix} 8 & -1 & -3 & -2 & -2 \\ -1 & 8 & -3 & -2 & -2 \\ -3 & -3 & 10 & -2 & -2 \\ -2 & -2 & -2 & 8 & -2 \\ -2 & -2 & -2 & -2 & 8 \end{bmatrix} \qquad \begin{bmatrix} 8 & -2 & -2 & -2 & -2 \\ -2 & 8 & -2 & -2 & -2 \\ -2 & -2 & 8 & -2 & -2 \\ -2 & -2 & -2 & 8 & -2 \\ -2 & -2 & -2 & -2 & 8 \end{bmatrix}$$

The diagonal entries make each row sum to zero.

Constructions: cyclic designs

This construction works if $b = v$. Label the treatments by the integers modulo v. Choose an initial block $\{i_1, i_2, \ldots, i_k\}$.
The next block is $\{i_1+1, i_2+1, \ldots, i_k+1\}$, and so on, with all arithmetic done modulo v.

1	2	3	4	5	6	7
2	3	4	5	6	7	1
4	5	6	7	1	2	3

1	2	3	4	5	6	7
2	3	4	5	6	7	1
3	4	5	6	7	1	2

−	1	2	4
1	0	6	4
2	1	0	5
4	3	2	0

−	1	2	3
1	0	6	5
2	1	0	6
3	2	1	0

The concurrence $\lambda_{ij} =$ the number of occurrences of $i - j$ in the table of differences. The design is balanced if every non-zero integer modulo v occurs equally often in the table of differences.

Construction: square lattice designs

This construction works if $v = k^2$.
Write out the treatments in a $k \times k$ square.

1	2	3
4	5	6
7	8	9

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

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

In the 1st replicate, the rows are blocks. In the 2nd replicate, the columns are blocks. If you want a 3rd replicate, write out a $k \times k$ Latin square and use its letters as blocks. For a 4th replicate, use a Latin square orthogonal to the first one, and so on.

1	4	7
2	5	8
3	6	9

1	2	3
4	5	6
7	8	9

1	2	3
6	4	5
8	9	7

1	2	3
5	6	4
9	7	8

When $r = k + 1$, the design is balanced.

Construction: projective planes

This construction works if $v = b = (k-1)^2 + k$.

Start with a square lattice design for $(k-1)^2$ treatments in $k(k-1)$ blocks of size $k - 1$.
Add a new treatment to every block in the first replicate.
Then do the same to the other replicates.
Add an extra block containing all the new treatments.

1	4	7
2	5	8
3	6	9
10	10	10

1	2	3
4	5	6
7	8	9
11	11	11

1	2	3
6	4	5
8	9	7
12	12	12

1	2	3
5	6	4
9	7	8
13	13	13

10
11
12
13

The final design is balanced.

Partially balanced designs: I

An association scheme on the treatments is a partition of the pairs of treatments into $s + 1$ associate classes, labelled $0, 1, \ldots, s$, subject to some conditions.
For the m-th associate class, define the $v \times v$ matrix A_m to have (i, j)-entry equal to

$$\begin{cases} 1 & \text{if } i \text{ and } j \text{ are } m\text{-th associates} \\ 0 & \text{otherwise.} \end{cases}$$

Conditions

(i) $A_0 = I$;
(ii) $A_0, A_1, \ldots, A_s$ are all symmetric;
(iii) $A_0 + A_1 + \cdots + A_s = J_v$;
(iv) $A_l A_m$ is a linear combination of $A_0, \ldots, A_s$, for $0 \leq l \leq s$ and $0 \leq m \leq s$.

A block design is partially balanced (with respect to this association scheme) if Λ is a linear combination of $A_0, \ldots, A_s$.

Partially balanced designs: II

Cyclic designs are partially balanced with respect to the cyclic association scheme, which has $s = \lfloor v/2 \rfloor$.

Treatments i and j are m-th associates if $i - j = \pm m$ modulo v.

Square lattice designs are partially balanced with respect to the Latin-square-type association scheme, which has $s = 2$.

Treatments i and j are first associates if $\lambda_{ij} = 1$; second associates otherwise.

Partially balanced designs: III

Suppose that $v = mn$ and the treatments are partitioned into m groups of size n. In the group-divisible association scheme, distinct treatments in the same group are first associates; treatments in different groups are second associates.

Let $v = 6$, $m = 3$ and $n = 2$, with groups $\{1, 4\}$, $\{2, 5\}$ and $\{3, 6\}$. The following design with $b = 4$ and $k = 3$ is group-divisible.

1	1	2	3
2	5	4	4
3	6	6	5

Laplacian matrix and information matrix

$B = ZZ^\top$ so $B^2 = ZZ^\top ZZ^\top = Z(Z^\top Z)Z^\top = Z(kI_b)Z^\top = kB$. Hence $\frac{1}{k}B$ is idempotent (and symmetric).

Put $Q = I - \frac{1}{k}B$. Then Q is also idempotent and symmetric.

Therefore $X^\top QX = X^\top Q^2 X = X^\top Q^\top QX = (QX)^\top (QX)$, which is non-negative definite.

$$X^\top QX = X^\top \left(I - \frac{1}{k}B \right) X = X^\top X - \frac{1}{k} X^\top ZZ^\top X = R - \frac{1}{k}\Lambda = \frac{1}{k}L = C,$$

where L is the Laplacian matrix and C is the information matrix.

So L and C are both non-negative definite.

Connectivity

All row-sums of L are zero,
so L has 0 as eigenvalue
on the all-1 vector.

The design is defined to be connected
if 0 is a simple eigenvalue of L.

From now on, assume connectivity.

Call the remaining eigenvalues *non-trivial*.
They are all non-negative.

Generalized inverse

Under the assumption of connectivity, the null space of L is spanned by the all-1 vector. The matrix $\frac{1}{v}J_v$ is the orthogonal projector onto this null space.

Then the Moore–Penrose generalized inverse L^- of L is defined by

$$L^- = \left(L + \frac{1}{v}J_v \right)^{-1} - \frac{1}{v}J_v.$$

Estimation

Since $Q = I - \frac{1}{k}B$,

$$QZ = Z - \frac{1}{k}(ZZ^\top)Z = Z - \frac{1}{k}Z(kI_b) = 0.$$

$$Y = X\tau + Z\beta + \varepsilon,$$

so

$$QY = QX\tau + QZ\beta + Q\varepsilon = QX\tau + Q\varepsilon,$$

and $\mathrm{Cov}(Q\varepsilon) = Q\sigma^2$, which is essentially scalar.

$$(QX)^\top QY = (QX)^\top QX\tau + (QX)^\top Q\varepsilon.$$

$$X^\top QY = X^\top QX\tau + X^\top Q\varepsilon = C\tau + X^\top Q\varepsilon.$$

Estimation, continued

$$X^\top QY = C\tau + X^\top Q\varepsilon.$$

We want to estimate contrasts $\sum_i x_i\tau_i$ with $\sum_i x_i = 0$.

In particular, we want to estimate all the simple differences $\tau_i - \tau_j$.

If x is a contrast and the design is connected then there is another contrast u such that $Cu = x$. Then

$$\sum_i x_i\tau_i = x^\top\tau = u^\top C\tau.$$

Least squares theory shows that the best linear unbiased estimator $u^\top C\hat{\tau}$ satisfies

$$u^\top X^\top QY = u^\top C\hat{\tau}.$$

Variance of estimates of contrasts

If $Cu = x$ then

$$\sum_i x_i\hat{\tau}_i = x^\top\hat{\tau} = u^\top C\hat{\tau} = u^\top X^\top QY.$$

The variance of this estimator is

$$u^\top X^\top Q(I\sigma^2)QXu = u^\top X^\top QXu\sigma^2 = u^\top Cu\sigma^2 = u^\top x\sigma^2 = x^\top C^- x\sigma^2.$$

$$C = \frac{1}{k}L \quad \text{so} \quad C^- = kL^-,$$

so the variance is $(x^\top L^- x)k\sigma^2$.

In particular, $\mathrm{Var}(\hat{\tau}_i - \hat{\tau}_j) = (L^-_{ii} + L^-_{jj} - 2L^-_{ij})k\sigma^2$.

Variance in balanced designs

In a balanced design, $r(k-1) = \lambda(v-1)$ and

$$\begin{aligned} L = krI_v - \Lambda &= krI_v - (rI_v + \lambda(J_v - I_v)) \\ &= r(k-1)I_v - \lambda(J_v - I_v) \\ &= \lambda(v-1)I_v - \lambda(J_v - I_v) \\ &= v\lambda\left(I_v - \frac{1}{v}J_v\right) \end{aligned}$$

so

$$L^- = \frac{1}{v\lambda}\left(I_v - \frac{1}{v}J_v\right)$$

and all variances of estimates of pairwise differences are the same, namely

$$\frac{2k}{v\lambda}\sigma^2 = \frac{2k(v-1)}{vr(k-1)}\sigma^2 = \frac{k(v-1)}{(k-1)v} \times \text{value in unblocked case.}$$

Variance in partially balanced designs

In a partially balanced design, L is a linear combination of A_0, …, A_s, and the conditions for an association scheme show that L^- is also a linear combination of $A_0, \ldots, A_s$, so there is a single pairwise variance for all pairs in the same associate class.

In particular, if $s = 2$ then there are precisely two concurrences and two pairwise variances, and all pairs with the same concurrence have the same pairwise variance. It can be shown that the smaller concurrence corresponds to the larger variance.

Warnings

This simple pattern does not hold for arbitrary block designs.

In general, pairs with the same concurrence may have different pairwise variances.

There are some designs where some pairs with low concurrence have smaller pairwise variance than some pairs with high concurrence.

Reparametrization of blocks

Put $\gamma_j = -\beta_j$ for $j = 1, \ldots, b$. Then

$$Y_\omega = \tau_{f(\omega)} - \gamma_{g(\omega)} + \varepsilon_\omega.$$

We can add the same constant to every τ_i and every γ_j without changing the model. So we cannot estimate $\tau_1, \ldots, \tau_v$.

But we can aspire to estimate differences such as $\tau_i - \tau_l$, $\gamma_j - \gamma_m$ and $\tau_i - \gamma_j$.

In matrix form,

$$Y = X\tau - Z\gamma + \varepsilon.$$

Least squares again

$$Y = X\tau - Z\gamma + \varepsilon = [X \mid -Z] \begin{bmatrix} \tau \\ \gamma \end{bmatrix} + \varepsilon.$$

The same theory as before shows that the best linear unbiased estimates of contrasts in $(\tau_1, \ldots, \tau_v, \gamma_1, \ldots, \gamma_b)$ satisfy

$$[X \mid -Z]^\top Y = [X \mid -Z]^\top [X \mid -Z] \begin{bmatrix} \hat{\tau} \\ \hat{\gamma} \end{bmatrix} = \tilde{L} \begin{bmatrix} \hat{\tau} \\ \hat{\gamma} \end{bmatrix},$$

where

$$\tilde{L} = \begin{bmatrix} X^\top \\ -Z^\top \end{bmatrix} [X \mid -Z] = \begin{bmatrix} X^\top X & -X^\top Z \\ -Z^\top X & Z^\top Z \end{bmatrix} = \begin{bmatrix} R & -N \\ -N^\top & kI_b \end{bmatrix}.$$

Variance again

Now let x be a contrast vector in $\mathbb{R}^{v+b}$.

If $\tilde{L}u = x$ then the best linear unbiased estimator of

$$x^\top \begin{bmatrix} \tau \\ \gamma \end{bmatrix} \quad \text{or} \quad u^\top \tilde{L} \begin{bmatrix} \tau \\ \gamma \end{bmatrix} \quad \text{is} \quad u^\top \begin{bmatrix} X^\top \\ -Z^\top \end{bmatrix} Y,$$

and the variance of this estimator is

$$(x^\top \tilde{L}^- x)\sigma^2.$$

In particular, $\mathrm{Var}(\hat{\tau}_i - \hat{\tau}_j) = (\tilde{L}^-_{ii} + \tilde{L}^-_{jj} - 2\tilde{L}^-_{ij})\sigma^2$.