Laplacian eigenvalues and optimality: I. Block designs

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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;),
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Mathematicians and statisticians

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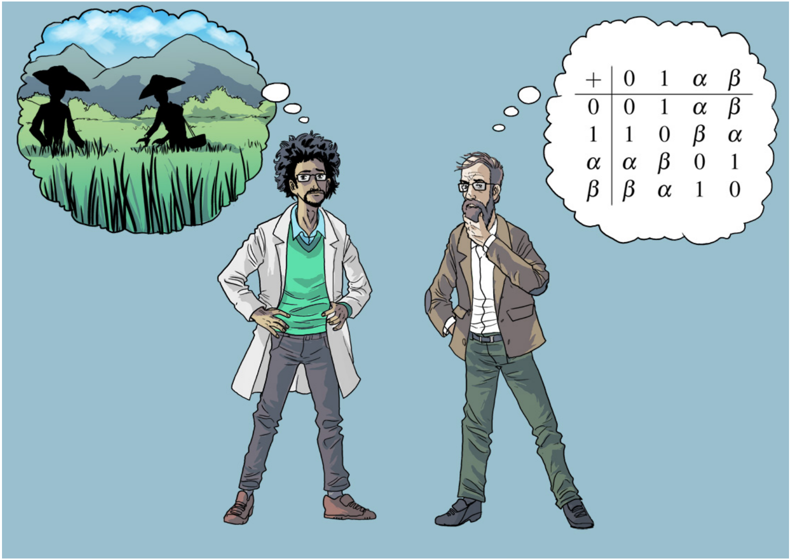
This comment refers to his years at the Indian Statistical Institute.

Mathematicians and statisticians



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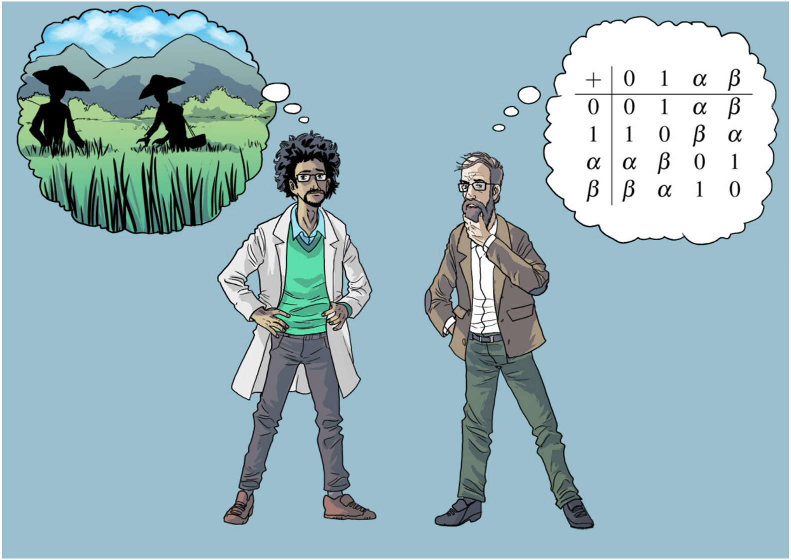


Thanks to Neill Cameron for this picture.

Outline

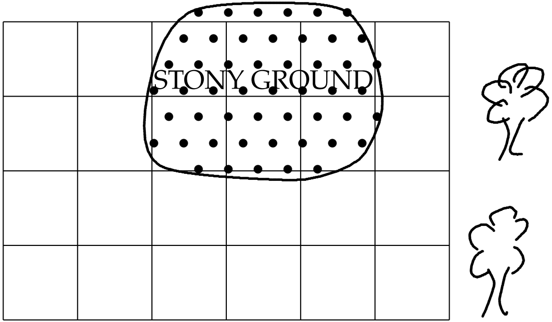
1. Experiments in blocks.
2. Complete-block designs.
3. Incomplete-block designs.
4. Matrix formulae.
5. Constructions.
6. Laplacian matrix and information matrix.
7. Estimation and variance.
8. Reparametrization.

Section 1

Experiments in blocks.

An experiment in a field

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



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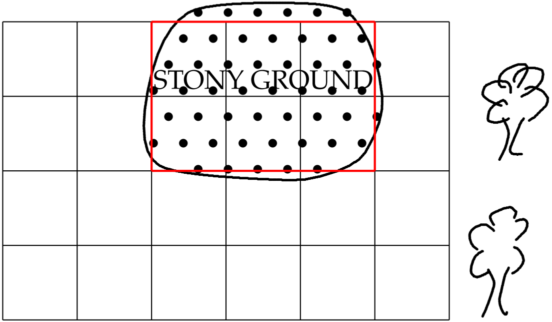

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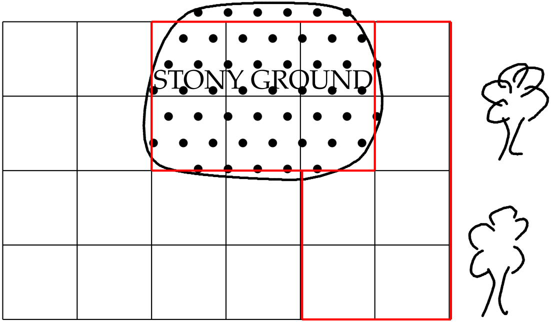

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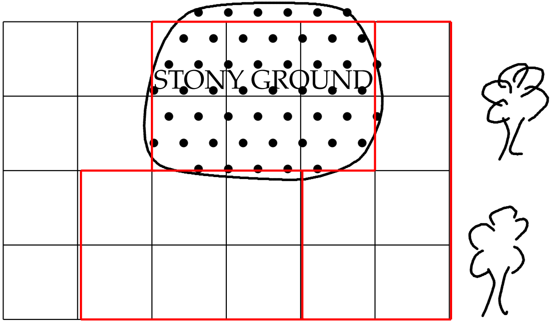

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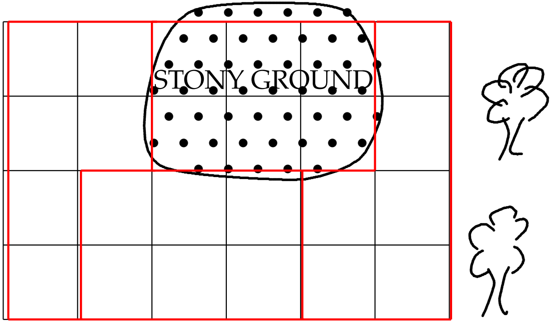

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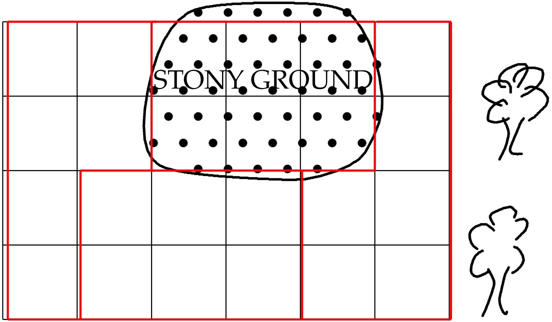

Partition the experimental units into homogeneous blocks and plant each variety on one plot in each block.

An experiment on people

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So there are 80 experimental units.
Each volunteer forms a block of size 2.

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The treatments are the 2 types of drink.

An experiment on diffusion of proteins

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

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days	5	10	numbers of cells	5
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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?

Section 2

Complete-block designs.

Complete-block designs: construction and randomization

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Statistical Model

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

We assume that the response Y_ω on plot ω satisfies:

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

$$\begin{aligned} \text{where} \quad \tau_i \quad & \text{is a constant depending on treatment } i, \\ \beta_j \quad & \text{is a constant depending on block } j, \end{aligned}$$

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

Estimating treatment differences

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The variance of this estimator is

$$\frac{2\sigma^2}{b}.$$

Residuals

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

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

Estimating variance

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

Estimating variance

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

Hence

$$\frac{\text{RSS}}{(b-1)(v-1)}$$

is an unbiased estimator of σ^2.

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   Then the variance of the best linear unbiased estimator of $\tau_i - \tau_j$ is
   $$\frac{2\sigma^2}{bs}.$$
3. In particular, if there is a single block and each treatment occurs r times then the variance of the best linear unbiased estimator of $\tau_i - \tau_j$ is
   $$\frac{2\sigma^2}{r}.$$

Section 3

Incomplete-block designs.

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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

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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 $vr = bk$.

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Proof.
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Comment
Statisticians tend to prefer equireplicate designs; biologists tend to prefer queen-bee designs.

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

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

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balanced (2-design)

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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 equireplicate and $r(k-1) = \lambda(v-1)$.

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If a binary design is balanced, with every pair of distinct treatments occuring together in λ blocks, then the design is equireplicate 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 $i = 1, \ldots, v$. □

Section 4

Matrix formulae.

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:

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Some column vectors

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

When the data are collected, they are usually written in a column vector of length bk:

$$Y = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_{bk} \end{pmatrix}.$$

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Similarly, define column vectors

$$\tau = \begin{pmatrix} \tau_1 \\ \tau_2 \\ \vdots \\ \tau_v \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_b \end{pmatrix} \quad \text{and} \quad \epsilon = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_{bk} \end{pmatrix}.$$

Some column vectors

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

When the data are collected, they are usually written in a column vector of length bk:

$$Y = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_{bk} \end{pmatrix}.$$

Similarly, define column vectors

$$\tau = \begin{pmatrix} \tau_1 \\ \tau_2 \\ \vdots \\ \tau_v \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_b \end{pmatrix} \quad \text{and} \quad \epsilon = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_{bk} \end{pmatrix}.$$

(Statisticians typically use column vectors rather than row vectors.)

Expressing the model in vector form

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

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Rewritten in vector form:

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

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

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

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The matrix X has bk rows (labelled by the experimental units) and v columns (labelled by the treatments);
the matrix Z has bk rows (labelled by the experimental units) and b columns (labelled by the blocks).

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

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

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

$$X = \begin{array}{c} \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

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

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

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

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

$$
Z = \begin{array}{c} \\ \end{array}
\begin{array}{cccc} B1 & B2 & B3 & B4 \end{array}
$$

$$
Z = \left[\begin{array}{cccc}
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1
\end{array}\right]
$$

Small example continued

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

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

More matrices

matrix	X	Z						
dimensions	$bk \times v$	$bk \times b$						

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

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matrix	X	Z	B					
dimensions	$bk \times v$	$bk \times b$	$bk \times bk$					

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

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

More matrices

matrix	X	Z	B	R				
dimensions	$bk \times v$	$bk \times b$	$bk \times bk$	$v \times v$				

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

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$$X^\top X = R = \text{diagonal matrix of treatment replications.}$$

More matrices

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

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

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

More matrices

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

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

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

$$X^\top X = R = \text{diagonal matrix of treatment replications.}$$

$$X^\top Z = N = \text{incidence matrix.}$$

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

$$NN^\top = \Lambda = \text{concurrence matrix.}$$

$$\begin{aligned} \lambda_{ij} &= \text{number of occurrences of } i \text{ and } j \text{ in the same block} \\ &= \text{concurrence of treatments } i \text{ and } j. \end{aligned}$$

More matrices

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

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

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$L = kR - \Lambda =$ Laplacian matrix;

More matrices

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

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

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

$$X^\top X = R = \text{diagonal matrix of treatment replications.}$$

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$$\begin{aligned} \lambda_{ij} &= \text{number of occurrences of } i \text{ and } j \text{ in the same block} \\ &= \text{concurrence of treatments } i \text{ and } j. \end{aligned}$$

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

Small example continued again

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

Small example continued again

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

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

Small example continued again

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

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

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

Small example: incidence matrix

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

Small example: incidence matrix

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

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

Small example: concurrence matrix

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

Small example: concurrence matrix

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

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

Small example: Laplacian matrix

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

Small example: Laplacian matrix

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

$$L = kR - \Lambda = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} \begin{array}{c} \begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{array} \\ \left[\begin{array}{rrrrrrrr} 4 & -1 & 0 & -1 & -1 & 0 & 0 & -1 \\ -1 & 4 & -1 & 0 & -1 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & -1 & -1 & 0 \\ -1 & 0 & -1 & 4 & 0 & 0 & -1 & -1 \\ -1 & -1 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & -1 & -1 & 0 & 0 & 2 & 0 \\ -1 & 0 & 0 & -1 & 0 & 0 & 0 & 2 \end{array}\right] \end{array}$$

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 $f(\omega) = j$.

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

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

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

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

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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 $b \geq v$.

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

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

$\square$

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

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

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

$$\begin{bmatrix} 8 & -2 & -2 & -2 & -2 \\ -2 & 8 & -2 & -2 & -2 \\ -2 & -2 & 8 & -2 & -2 \\ -2 & -2 & -2 & 8 & -2 \\ -2 & -2 & -2 & -2 & 8 \end{bmatrix}$$

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

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

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

$$\begin{bmatrix} 8 & -2 & -2 & -2 & -2 \\ -2 & 8 & -2 & -2 & -2 \\ -2 & -2 & 8 & -2 & -2 \\ -2 & -2 & -2 & 8 & -2 \\ -2 & -2 & -2 & -2 & 8 \end{bmatrix}$$

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

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

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

$$\begin{bmatrix} 8 & -2 & -2 & -2 & -2 \\ -2 & 8 & -2 & -2 & -2 \\ -2 & -2 & 8 & -2 & -2 \\ -2 & -2 & -2 & 8 & -2 \\ -2 & -2 & -2 & -2 & 8 \end{bmatrix}$$

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

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

$$\begin{bmatrix} 8 & -2 & -2 & -2 & -2 \\ -2 & 8 & -2 & -2 & -2 \\ -2 & -2 & 8 & -2 & -2 \\ -2 & -2 & -2 & 8 & -2 \\ -2 & -2 & -2 & -2 & 8 \end{bmatrix}$$

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.

Section 5

Constructions.

Construction: cyclic designs

This construction works if $b = v$.

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This construction works if $b = v$. Label the treatments by the integers modulo v. Choose an initial block $\{i_1, i_2, \ldots, i_k\}$.

Construction: 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.

Construction: cyclic designs

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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

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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
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$-$	1	2	4
1	0	6	4
2	1	0	5
4	3	2	0

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2	1	0	6
3	2	1	0

The concurrence $\lambda_{ij} =$ the number of occurrences of $i - j$ in the table of differences.

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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 $v = k^2$.

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Write out the treatments in a $k \times k$ square.

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Write out the treatments in a $k \times k$ square.

1	2	3
4	5	6
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A	B	C
B	C	A
C	A	B

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.

1 2 3	4 5 6	7 8 9

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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.
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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

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

Construction: projective planes

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2	5	8
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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.

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

1	2	3
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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

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

1	4	7
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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 set of v^2 ordered 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

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

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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 $s = \lfloor v/2 \rfloor$.

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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.

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Warnings about terminology

Balanced incomplete-block designs are the special case of partially balanced incomplete-block designs with $s = 1$.

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If an incomplete-block design is not balanced then this does not imply that it is partially balanced.

Section 6

Laplacian matrix and information matrix.

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$B = ZZ^\top$ so $B^2 = ZZ^\top ZZ^\top = Z(Z^\top Z)Z^\top = Z(kI_b)Z^\top = kB.$

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It has rank $b(k-1)$.

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

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

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So L and C are both non-negative definite.

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so L has 0 as eigenvalue
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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.

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

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

Section 7

Estimation and variance.

Covariance matrices in general

If

$$U = \begin{pmatrix} U_1 \\ U_2 \\ \vdots \\ U_n \end{pmatrix}$$

is a random vector of length n, then its variance-covariance matrix $\mathrm{Cov}(U)$ is the $n \times n$ real symmetric matrix whose diagonal entries are the variances $\mathrm{Var}(U_1), \dots, \mathrm{Var}(U_n)$ and whose (i, j)-off-diagonal entry is the covariance $\mathrm{Cov}(U_i, U_j)$. It is non-negative definite.

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Theorem

If M is a $m \times n$ real matrix then MU is a random vector of length m and $\mathrm{Cov}(MU) = M\,\mathrm{Cov}(U)M^\top$.

Covariance matrices for our random vectors

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

Everything in $X\tau$ and $Z\beta$ is a constant, so

$$\text{Cov}(Y) = \text{Cov}(\epsilon) = I\sigma^2.$$

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(The last step was one of our initial assumptions.)

Estimation

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

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

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so

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

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

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and $\mathrm{Cov}(Q\varepsilon) = Q\,\mathrm{Cov}(\varepsilon)Q^\top = Q\sigma^2$, 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

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

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Variance of estimates of contrasts

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We should like all such variances to be as small as possible.

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

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

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Comment

Matrix inversion was not easy in the pre-computer age.
One reason for the introduction of balanced incomplete-block designs and partially balanced incomplete-block designs was that it was relatively easy to calculate L^- and hence to calculate the pairwise variances.

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.

Residuals

If the block design is connected,
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As before, the residual on experimental unit ω is

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

and the residual sum of squares RSS is

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Hence

$$\frac{\mathrm{RSS}}{bk - b - v + 1}$$

is an unbiased estimator of σ^2.

Section 8

Reparametrization.

Non-standard reparametrization of blocks

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

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

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Recall that R is the diagonal matrix of treatment replications and that N is the incidence matrix.

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