Incomplete-block designs and Laplacian eigenvalues

R. A. Bailey
University of St Andrews / QMUL (emerita)
rab@mcs.st-and.ac.uk, r.a.bailey@qmul.ac.uk

Combinatorics, Algebra, and More:
Conference for Peter Cameron,
Queen Mary, University of London,
July 2013

August 2007: Ambleside

Peter Cameron’s 60th birthday conference
What has he been doing since then?

April 2008: Christchurch, New Zealand

As London Mathematical Society Forder lecturer,
he travelled from one end of New Zealand to the other,
giving lectures in every university town.

September 2008: Torrita di Siena, Tuscany

Visiting Dan Hughes

Dan Hughes

Dan Hughes was professor of Pure Mathematics
at Westfield College, University of London,
then at Queen Mary and Westfield College.
He was instrumental in bringing Peter to Queen Mary and
Westfield College in 1986
and in setting up the Monday Pure Mathematics pro-seminar.
He retired in 1992 and died on 19 October 2012.

January 2009: Perth, Western Australia

“Are you the reviewer for the West Australian?”
Conference on Combinatorics, Computing and Group Theory
to celebrate Cheryl Praeger’s 60th birthday.
June 2009: Fife Coast Path

Working in St Andrews as external examiner for a PhD.

July 2010: in the Chilterns

Doing the research for Thursday’s walk

August 2010: Kerala

Onam lunch on holiday after the conference Recent Trends in Graph Theory and Combinatorics at Cochin.

June 2011: Kloster Irsee, Germany

Conference on Finite Geometries

September 2011: Cambridge

Working hard at the Design and Analysis of Experiments programme at the Isaac Newton Institute.

April 2012: Lisboa

Trying out the local furniture during a joint visit (PJC to Centro de Álgebra da Universidade de Lisboa, RAB to Universidade Nova)
July 2012: Torre, near Covilhã, Portugal

Bunking off during a session at Workshop on Statistics, Mathematics and Computation / Portuguese-Polish Workshop on Biometry

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.

<table>
<thead>
<tr>
<th>Blocks</th>
<th>( b )</th>
<th>( k )</th>
<th>Treatments</th>
<th>( v )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Housewives</td>
<td>12</td>
<td>4</td>
<td>Detergents</td>
<td>16</td>
</tr>
</tbody>
</table>

How should I choose a block design for these values of \( b \), \( v \) and \( k \)?

What makes a block design good?

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

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

<table>
<thead>
<tr>
<th>Blocks</th>
<th>( b )</th>
<th>( k )</th>
<th>Treatments</th>
<th>( v )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 1 1 1 1 2 2</td>
<td>1 1 1 1 2 2 2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 3 3 3 4 4 4</td>
<td>2 3 4 4 5 5 5</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

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

<table>
<thead>
<tr>
<th>Blocks</th>
<th>( b )</th>
<th>( k )</th>
<th>Treatments</th>
<th>( v )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 1 1 1 1 1 1</td>
<td>1 1 1 1 1 1 1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 4 6 8 10 12 14</td>
<td>2 4 6 8 10 12 14</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3 5 7 9 11 13 15</td>
<td>3 5 7 9 11 13 15</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Replications differ by \( \leq 1 \) 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.

Two designs with \( v = 7 \), \( b = 7 \), \( k = 3 \): which is better?

<table>
<thead>
<tr>
<th>Blocks</th>
<th>( b )</th>
<th>( k )</th>
<th>Treatments</th>
<th>( v )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 2 3 4 5 6 7</td>
<td>1 2 3 4 5 6 7</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 3 4 5 6 7 1</td>
<td>2 3 4 5 6 7 1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 5 6 7 1 2 3</td>
<td>4 5 6 7 1 2 3</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A binary design is balanced if every pair of distinct treatments occurs together in the same number of blocks.
Experimental units and incidence matrix

There are $bk$ experimental units. If $\omega$ is an experimental unit, put

$$f(\omega) = \text{treatment on } \omega$$
$$g(\omega) = \text{block containing } \omega.$$ 

For $i = 1, \ldots, v$ and $j = 1, \ldots, b$, let

$$n_{ij} = |\{\omega : f(\omega) = i \text{ and } g(\omega) = j\}|$$

be the number of experimental units in block $j$ which have treatment $i$. The $v \times b$ incidence matrix $N$ has entries $n_{ij}$.

Levi graph

The Levi graph $\tilde{G}$ of a block design $\Delta$ has

- one vertex for each treatment,
- one vertex for each block,
- one edge for each experimental unit, with edge $\omega$ joining vertex $f(\omega)$ to vertex $g(\omega)$. 

It is a bipartite graph, with $n_{ij}$ edges between treatment-vertex $i$ and block-vertex $j$.

Concurrence graph

The concurrence graph $G$ of a block design $\Delta$ has

- one vertex for each treatment,
- one edge for each unordered pair $\alpha, \omega$, with $\alpha \neq \omega$, $g(\alpha) = g(\omega)$ and $f(\alpha) \neq f(\omega)$; this edge joins vertices $f(\alpha)$ and $f(\omega)$. 

There are no loops.

If $i \neq j$ then the number of edges between vertices $i$ and $j$ is

$$\lambda_{ij} = \sum_{s=1}^{b} n_{is} n_{sj}$$

this is called the concurrence of $i$ and $j$, and is the $(i,j)$-entry of $\Lambda = NN^T$. 

Example 1: $v = 4$, $b = k = 3$

Example 2: $v = 8$, $b = 4$, $k = 3$

Example 1: $v = 4$, $b = k = 3$

Example 2: $v = 8$, $b = 4$, $k = 3$
Example 2: \( v = 8, b = 4, k = 3 \)

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

Laplacian matrices

The Laplacian matrix \( L \) of the concurrence graph \( G \) is a \( v \times v \) matrix with \((i,j)\)-entry as follows:
- \( l_{ij} = - (\text{number of edges between } i \text{ and } j) \),
- \( l_{ii} = \text{valency of } i = \sum_j l_{ij} \).

The Laplacian matrix \( L \) of the Levi graph \( G \) is a \((v+b) \times (v+b)\) matrix with \((i,j)\)-entry as follows:
- \( l_{ii} = \text{valency of } i \)
- \( l_{ij} = k \) if \( i \) is a block
- \( l_{ij} = - (\text{number of edges between } i \text{ and } j) \) if \( i \) is a treatment
- \( l_{ij} = 0 \) if \( i \) and \( j \) are both blocks
- \( l_{ij} = -n_i \) if \( i \) is a treatment and \( j \) is a block, or vice versa.

Connectivity

All row-sums of \( L \) and of \( L \) are zero, so both matrices have 0 as eigenvalue on the appropriate all-1 vector.

Theorem

The following are equivalent.
1. 0 is a simple eigenvalue of \( L \);
2. \( G \) is a connected graph;
3. \( G \) is a connected graph;
4. 0 is a simple eigenvalue of \( L \);
5. the design \( X \) is connected in the sense that all differences between treatments can be estimated.

From now on, assume connectivity.

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

Estimation and variance

We measure the response \( Y_\omega \) on each experimental unit \( \omega \).

If experimental unit \( \omega \) has treatment \( i \) and is in block \( m \) \( if(\omega) = i \) and \( g(\omega) = m \), then we assume that
\[
Y_\omega = \tau_i + \beta_m + \text{random noise}.
\]

We want to estimate contrasts \( \sum x_i \tau_i \) with \( \sum x_i = 0 \).

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

Put \( V_\nu = \text{variance of the best linear unbiased estimator for } \tau_i - \tau_j \).

We want all the \( V_\nu \) to be small.
How do we calculate variance?

Theorem
Assume that all the noise is independent, with variance $\sigma^2$.
If $\sum x_i = 0$, then the variance of the best linear unbiased estimator of $\sum x_i y_i$ is equal to
\[(x^\top (L^{-1} x))^2 \cdot \sigma^2.
\]
In particular, the variance of the best linear unbiased estimator of the simple difference $x_i - x_j$ is
\[V_{ij} = (L^{-1} L^{-1} - 2L^{-1}ij) \cdot \sigma^2.
\]
(This follows from assumption $\tau_i - \tau_j$ is 
$\beta_i - \beta_j$, appropriately labelled.)

Electrical networks

We can consider the concurrence graph $G$ as an electrical network with a 1-ohm resistance in each edge.
Current flows in the network, according to these rules.
1. Ohm’s Law:
   - In every edge, voltage drop = current $\times$ resistance $\times$ current.
2. Kirchhoff’s Voltage Law:
   - The total voltage drop from one vertex to any other vertex is the same no matter which path we take from one to the other.
3. Kirchhoff’s Current Law:
   - At every vertex which is not connected to the battery, the total current coming in is equal to the total current going out.
Find the total current $I$ from $i$ to $j$, then use Ohm’s Law to define the effective resistance $R_{ij}$ between $i$ and $j$ as $\frac{1}{I}$.

Example 2 calculation: $v = 8$, $b = 4$, $k = 3$

$V = 23$ $I = 24$ $R = \frac{23}{24}$

\[V_{ij} = (L^{-1} L^{-1} - 2L^{-1}ij) \cdot \sigma^2.
\]

Or we can use the Levi graph

$V_{ij} = (L^{-1} L^{-1} - 2L^{-1}ij) \cdot \sigma^2.$

Effective resistances are easy to calculate without matrix inversion if the graph is sparse.

If $i$ and $j$ are treatment vertices in the Levi graph $\hat{G}$ and $\hat{R}_{ij}$ is the effective resistance between them in $\hat{G}$ then

$V_{ij} = \hat{R}_{ij} \times \sigma^2.$

The variance of the best linear unbiased estimator of the simple difference $\tau_i - \tau_j$ is
$V_{ij} = (L^{-1} L^{-1} - 2L^{-1}ij) \cdot \sigma^2.$

(Or $\beta_i - \beta_j$, appropriately labelled.)

(This follows from assumption $\tau_i - \beta_i$ is random noise.
by using standard theory of linear models.)
What about the Levi graph?

Example 2 yet again: \( v = 8, b = 4, k = 3 \)

Average pairwise variance

The variance of the best linear unbiased estimator of the simple difference \( \tau_i - \tau_j \) is

\[
V_{ij} = \left( L_{ii} - 2L_{ij} - 2L_{jj} \right) k \sigma^2.
\]

Putting \( \bar{V} = \text{average value of the } V_{ij} \) Then

\[
\bar{V} = \frac{2k \sigma^2 \text{Tr}(L^{-1})}{v - 1} = 2k \sigma^2 \times \frac{1}{\text{harmonic mean of } \theta_1, \ldots, \theta_{v-1}},
\]

where \( \theta_1, \ldots, \theta_{v-1} \) are the nontrivial eigenvalues of \( L \).

Optimality

The design is called
- **A-optimal** if it minimizes the average of the variances \( V_{ij} \);
  —equivalently, it maximizes the harmonic mean of the Laplacian matrix \( L \);
- **D-optimal** if it minimizes the volume of the confidence ellipsoid for \( (\tau_1, \ldots, \tau_v) \);
  —equivalently, it maximizes the geometric mean of the non-trivial eigenvalues of the Laplacian matrix \( L \);
- **E-optimal** if it minimizes the largest value of \( x^T L^{-1} x / x^T x \);
  —equivalently, it maximizes the minimum nontrivial eigenvalue \( \theta_1 \) of the Laplacian matrix \( L \);

over all block designs with block size \( k \) and the given \( v \) and \( b \).

D-optimality: spanning trees

A spanning tree for the graph is a collection of edges of the graph which form a tree (connected graph with no cycles) and which include every vertex.


\[
\text{product of non-trivial eigenvalues of } L = v \times \text{number of spanning trees}.
\]

So a design is D-optimal if and only if its concurrence graph \( G \) has the maximal number of spanning trees.

This is easy to calculate by hand when the graph is sparse.

What about the Levi graph?

Theorem (Gaffke)

Let \( G \) and \( \tilde{G} \) be the concurrence graph and Levi graph for a connected incomplete-block design for \( v \) treatments in \( b \) blocks of size \( k \).

Then the number of spanning trees for \( G \) is equal to \( k^{v-b-1} \times \text{number of spanning trees for } \tilde{G} \).

So a block design is D-optimal if and only if its Levi graph maximizes the number of spanning trees.

If \( v \geq b + 2 \) it is easier to count spanning trees in the Levi graph than in the concurrence graph.

Example 2 one last time: \( v = 8, b = 4, k = 3 \)

Optimality

The design is called
- **A-optimal** if it minimizes the average of the variances \( V_{ij} \);
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  —equivalently, it maximizes the geometric mean of the non-trivial eigenvalues of the Laplacian matrix \( L \);
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So a design is D-optimal if and only if its concurrence graph \( G \) has the maximal number of spanning trees.

This is easy to calculate by hand when the graph is sparse.
**E-optimality: the cutset lemma**

A design is E-optimal if it maximizes the smallest non-trivial eigenvalue $\theta_1$ of the Laplacian $L$ of the concurrence graph $G$.

**Lemma**

Let $G$ have an edge-cutset of size $c$
(set of $c$ edges whose removal disconnects the graph)
whose removal separates the graph into components of sizes $m$ and $n$.
Then

$$\theta_1 \leq c \left( \frac{1}{m} + \frac{1}{n} \right).$$

If $c$ is small but $m$ and $n$ are both large, then $\theta_1$ is small.
There is a similar result for vertex-cutsets.

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**Can we use the Levi graph to find E-optimal designs?**

For binary designs with equal replication, $\theta_1(L)$ is a monotonic increasing function of $\theta_1(\tilde{L})$.

For general block designs, we do not know if we can use the Levi graph to investigate E-optimality.

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**Timeline: 2007–2008**

- RAB talked about these results in the QMUL Combinatorics Study Group, …
- … and extended them to larger block size $k$, …
- … and realised that pairwise variance is proportional to effective resistance in the concurrence graph.
- PJC found lots of connections with other uses of the Laplacian eigenvalues, especially the smallest (which gives E-optimality).
- In 2008, we discovered that Tjur had published a paper in 1991 which showed that pairwise variance is the same as effective resistance in the Levi graph (so he had given an earlier proof for A-optimality when $k = 2$).
- RAB and PJC assumed that the Levi graph was more complicated than the concurrence graph and so did not pursue this.

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**Timeline: 2009–2010**

- PJC gave an invited talk on this at the 2009 British Combinatorial Conference in St Andrews.
- Lowell Beineke immediately asked us to write a chapter about this for a book that he and Robin Wilson were editing.
- PJC and RAB agreed, but did nothing for two years.
- In late 2010, Brian Cullis asked RAB (on a visit to CSIRO) about optimality of block designs with large $v$ and average replication $\bar{r}$ much less than 2.
- RAB found the A-optimal designs for very low $\bar{r}$.

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**E-optimality when $v = 2b + 1$ and $k = 3$**

The Levi graph has $3b + 1$ vertices and $3b$ edges, so it is a tree.

\[
\theta_1 \leq 2 \left( \frac{1}{5} + \frac{1}{10} \right) \quad \theta_1 \geq 1
\]

The only E-optimal designs are the queen-bee designs.
### Timeline: 2011–2012

- At the Isaac Newton Institute in 2011, PJC and RAB wrote the chapter, and realised that the Levi graph gives simpler calculations of effective resistance when \( k \geq 3 \).
- Also at INI, RAB re-read Gaffke’s 1981 paper as part of another collaboration, and discovered that the Levi graph is simpler for counting spanning trees when \( v \geq b + 2 \).
- In June 2012, PJC and RAB gave an intensive short course on this stuff at the London Taught Courses Centre.
- RAB used the Levi graph to find D-optimal block designs when \( \bar{r} << 2 \).

### Timeline: 2013

- At the Spring Research Conference in Los Angeles in June 2013, (Harvey) Xianggui Qu asked RAB if the graphical method can be used for row–column designs with \( \bar{r} << 2 \).
- “No, because that trick with changing signs works when you have two factors but cannot be extended to three or more. Tjur pointed that out in his paper.”
- After an overnight flight North of the Arctic Circle at the summer solstice, absolutely dog-tired . . .
- . . . Aha! There is a third type of graph, and maybe that would work.

### Example 1 finally: \( v = 4, b = k = 3 \)

The Levi graph has vertices for blocks and vertices for treatments.

\[
\begin{array}{ccc}
1 & 2 & 1 \\
3 & 3 & 2 \\
4 & 4 & 2 \\
\end{array}
\]

The third type of graph has vertices for treatments, blocks and experimental units.

\[
\begin{array}{ccc}
4 \\
1 & 2 \\
3 \\
\end{array} \quad \begin{array}{ccc}
4 \\
1 & 2 \\
3 \\
\end{array}
\]

### The third type of graph

- Effective resistance in the third type of graph is twice that of effective resistance in the Levi graph.
- Each edge removed from the Levi graph to make a spanning tree gives a choice of two edges to remove from the third type of graph to make a spanning tree.
- The third type of graph can be extended to row–column designs (with four different types of vertices);
- in which guise it has been successfully used by Brendan McKay for deciding isomorphism of row–column designs;
- how about for investigating row–column designs?