Laplacian eigenvalues and optimality:
III. Designs, graphs and optimality

R. A. Bailey and Peter J. Cameron
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**Block designs**

A block design $\Delta$ consists of
- a set of $bk$ experimental units (also called plots), partitioned into $b$ blocks of size $k$;
- a set of $v$ treatments;
- a function $f$ from the experimental units onto the set of treatments, so that $f(\omega)$ denotes the treatment applied to experimental unit $\omega$.

$g(\omega)$ denotes the block containing $\omega$.

$N_{ij}$ denotes the number of occurrences of treatment $i$ in block $j$.

For treatments $i$ and $l$, the concurrence of $i$ and $l$ is

$$\lambda_{il} = \sum_{j=1}^{b} N_{ij}N_{lj}.$$  

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**Outline**

1. Two graphs associated with a block design.
2. Laplacian matrices.
3. Estimation and variance.
4. Resistance distance.
5. Spanning trees.
7. Some optimal designs.
8. Designs with very low replication.

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**Section 1**

Two graphs associated with a block design.

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**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 $j$.

Friedrich W. Levi was a German Jewish mathematician who had to leave Nazi Germany in the 1930s. He moved to India, where he worked at the Indian Statistical Institute with R. C. Bose. He invented this graph to describe a block design. Later authors named it after him. Some other authors call it the incidence graph.

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

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

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

\[
\begin{array}{cccc}
1 & 2 & 3 & 4 \\
2 & 3 & 4 & 1 \\
5 & 6 & 7 & 8 \\
\end{array}
\]
The concurrence graph $G$ of a block design $\Delta$ has

- one vertex for each treatment,
- one edge for each unordered pair $\alpha, \omega$, with $\alpha \neq \omega$,
  
  \[ g(\alpha) = g(\omega) \text{ and } f(\alpha) \neq f(\omega), \]

  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

\[ \lambda_{ij} = \sum_{\alpha=1}^{b} N_{\alpha,i} N_{\alpha,j}; \]

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

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

<table>
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</tr>
<tr>
<td>3</td>
<td>4</td>
<td>2</td>
</tr>
</tbody>
</table>

Levi graph

Concurrence graph

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

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<th>1</th>
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<th>3</th>
<th>4</th>
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</thead>
<tbody>
<tr>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
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</table>

Levi graph

Concurrence graph

Example 3: $v = 15, b = 7, k = 3$

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<th>5</th>
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<td>9</td>
<td>10</td>
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<td>12</td>
<td>13</td>
<td>14</td>
<td>15</td>
<td></td>
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</tbody>
</table>

Laplacian matrix of the concurrence graph

The Laplacian matrix $L$ of the concurrence graph $G$ is a $v \times v$ matrix with $(i, j)$-entry as follows:

- if $i \neq j$ then
  
  \[ L_{ij} = -(\text{number of edges between } i \text{ and } j) = -\lambda_{ij}; \]

- $L_{ii} =$ valency of $i = \sum_{j=1}^{v} \lambda_{ij}$.

The off-diagonal entries are the same as those of $-\Lambda$.

The diagonal entries make each row sum to zero.

So the graph-theoretic definition of Laplacian matrix gives us exactly the Laplacian matrix $L$ that we defined before.
### Laplacian matrix of the Levi graph

The Laplacian matrix \( \tilde{L} \) of the Levi graph \( \tilde{G} \) is a \((v + b) \times (v + b)\) matrix with \((i,j)\)-entry as follows:

\[
\tilde{L}_{ij} = \begin{cases} 
\ell & \text{if } i \text{ is a block} \\
\tau_i & \text{if } i \text{ is a treatment} \\
0 & \text{if } i \neq j \text{ then } \tilde{L}_{ij} = -(\text{number of edges between } i \text{ and } j) \\
-N_j & \text{if } i \text{ is a treatment and } j \text{ is a block, or vice versa.}
\end{cases}
\]

So \( \tilde{L} = \begin{bmatrix} R & -N \\ -N^T & kI_b \end{bmatrix} \),

which is exactly the same as our previous definition of \( \tilde{L} \).

### Connectivity

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

**Theorem**

The following are equivalent.

1. \( \tilde{G} \) is a connected graph;
2. \( G \) is a connected graph;
3. \( G \) is a connected graph;
4. \( \tilde{G} \) is a simple eigenvalue of \( L \);
5. the design \( \Delta \) 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.

### Section 3

**Variance: why does it matter?**

We want to estimate all the simple differences \( \tau_i - \tau_j \).

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

The length of the 95\% confidence interval for \( \tau_i - \tau_j \) is proportional to \( \sqrt{V_{ij}} \).

(If we always present results using a 95\% confidence interval, our interval will contain the true value in 19 cases out of 20.)

The smaller the value of \( V_{ij} \), the smaller is the confidence interval, the closer is the estimate to the true value (on average), and the more likely are we to detect correctly which of \( \tau_i \) and \( \tau_j \) is bigger.

We can make better decisions about new drugs, about new varieties of wheat, about new engineering materials ... if we make all the \( V_{ij} \) small.

### How do we calculate variance?

**Theorem**

Assume that all the noise is independent, with variance \( \sigma^2 \).

If \( \sum \tau_i = 0 \), then the variance of the best linear unbiased estimator of \( \sum \tau_i \) is equal to \( (\sum \tau_i)^2 \sum \sigma^2 \).

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

\[
V_{ij} = \left( L_{ii}^{-1} + L_{jj}^{-1} - 2L_{ij}^{-1} \right) \sigma^2.
\]

**Comment**

All vectors in this lecture are column vectors.

### . . . Or we can use the Levi graph

**Theorem**

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

\[
V_{ij} = \left( L_{ii}^{-1} + L_{jj}^{-1} - 2L_{ij}^{-1} \right) \sigma^2.
\]
### Section 4

Resistance distance.

### Electrical networks: variance and resistance

We can consider the concurrence graph $G$ as an electrical network, and define the resistance distance $R_{ij}$ between any pair of distinct vertices $i$ and $j$.

**Comment**

The resistance distance $R_{ij}$ was written as $R(i, j)$ in Lecture II.

**Theorem**

The resistance distance $R_{ij}$ between vertices $i$ and $j$ in $G$ is

$$R_{ij} = \left( L_x + L_y - 2L_{xy} \right).$$

So

$$V_y = R_{ij} \times k\sigma^2.$$

Resistance distances are easy to calculate without matrix inversion if the graph is sparse.

### Comments on calculating resistance distance

If I want to calculate the resistance distance between vertices $i$ and $j$, I start by assigning voltage $[0]$ at vertex $i$.

Then I send a current $x$ along one of the edges out of $i$.

I am not a physicist, so I show the electricity running uphill, and the end of that edge gets allocated voltage $[x]$.

I apply one of Kirchoff’s Laws at each vertex, and the other of Kirchoff’s Laws in each edge.

When I reach vertex $j$, there are some equations to solve, enabling me to give the voltage $[V]$ at vertex $j$ and then calculate the total current $I$ flowing from vertex $i$ to vertex $j$.

Ohm’s Law gives

$$V = IR,$$

which I use to calculate $R_{ij}$ as $V/I$.

### Example calculation: $v = 12, b = 6, k = 3$

If $i$ and $j$ are treatment vertices in the Levi graph $G$, and $R_{ij}$ is the resistance distance between them in $G$ then

$$V_0 = R_{ij} \times e^2.$$
Example 2 yet again: $v = 8, b = 4, k = 3$

\[ V = 23 \]
\[ I = 8 \]
\[ R = \frac{23}{8} \]

Levi graph for the example before last

Resistance calculation for previous slide

\[ \tilde{R}_{12} = \tilde{R}_{1B} + \tilde{R}_{B2} \]

because resistances in series are simply added together.

But \( \tilde{R}_{12} = 1 \), and so \( \tilde{R}_{12} = \tilde{R}_{1B} + 1 \).

There are two disjoint paths from vertex 1 to vertex B, of lengths 5 and 7. These have resistances 5 and 7 in parallel, so \( \tilde{R}_{1B} = \frac{1}{5} + \frac{1}{7} = \frac{1}{35} + \frac{1}{35} = \frac{35}{12} \).

Therefore \( \tilde{R}_{12} = \frac{35}{12} + 1 = \frac{47}{12} \).

Concurrence graph or Levi graph?

For hand calculation when the graphs are sparse, or for calculations for ‘general’ graphs with variable \( v \), it may be simpler to use the Levi graph rather than the concurrence graph if \( k \geq 3 \).

Section 5

Spanning trees in the two graphs

\[ \text{Spanning trees.} \]

**Theorem**

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 \( \tilde{G} \) is equal to \( k^{b-v+1} \) times the number of spanning trees for \( G \).
Spanning trees in the two graphs: proof

Proof.
Let $t$ and $\tilde{t}$ be the number of spanning trees for $G$ and $\tilde{G}$ respectively. Then

\[ t = \det L_1 = \det(\xi R_1 - N_1 N_1^\top) \quad \text{and} \quad \tilde{t} = \det \tilde{L}_1, \]

where the subscript $1$ denotes the removal of the row and column corresponding to treatment $1$.

\[
\begin{align*}
\det L_1 &= \det \begin{bmatrix} R_1 & -N_1 \\ -N_1^\top & kI_b \end{bmatrix} = \det \begin{bmatrix} R_1 - k^{-1}(N_1 N_1^\top) & -N_1 \\ -N_1 & kI_b \end{bmatrix} \\
&= \det \begin{bmatrix} k^{-1}L_1 - N_1 \\ 0 & kI_b \end{bmatrix} = k^{-v+1} \det L_1 \times k^2 \\
\text{so} \quad \tilde{t} = \det \tilde{L}_1 = k^{v+1} \det L_1 = k^{v+1}t.
\end{align*}
\]

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

<table>
<thead>
<tr>
<th>Levi graph</th>
<th>concurrence graph</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 spanning trees</td>
<td>216 spanning trees</td>
</tr>
</tbody>
</table>

Optimality: Average pairwise variance

The variance of the best linear unbiased estimator of the simple difference $\tau_1 - \tau_i$ is

\[ V_\theta = \left( L_{ii} + L_{ij} \right) k\sigma^2 = R_k k\sigma^2. \]

We want all of the $V_\theta$ to be small.

\[
\frac{1}{2k} \sum_{i,j} V_{ij} = (v-1) \sum_i L_{ii} - \sum_{i<j} L_{ij} \\
= \sigma \sum_i L_{ii} \quad \text{because the row sums of } L \text{ are zero} \\
= \sigma \text{Trace}(L) \\
= v \left( \frac{1}{\theta_1} + \cdots + \frac{1}{\theta_{v-1}} \right),
\]

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

Optimality: Average pairwise variance, continued

The variance of the best linear unbiased estimator of the simple difference $\tau_1 - \tau_i$ is $V_\theta$. We want all of the $V_\theta$ to be small.

Put $\bar{V} = \text{average value of the } V_\theta$. Then

\[
\bar{V} = \frac{\sum_{t \in \mathcal{G}(G \cup \mathcal{P})} V_{ii}}{\binom{v}{2}} = \frac{k\sigma^2}{\binom{v}{2}} \times v \left( \frac{1}{\theta_1} + \cdots + \frac{1}{\theta_{v-1}} \right),
\]

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

Measures of optimality.
A block design is called **A-optimal** if it minimizes the average of the variances $V_{ij}$; 
—equivalently, it maximizes the harmonic mean of the nontrivial eigenvalues of the Laplacian matrix $L$, over all block designs with block size $k$ and the given $v$ and $b$.

### A-Optimality

$$\hat{\theta}_1, \ldots, \hat{\theta}_{v-1}$$ are the nontrivial eigenvalues of $L$.

If the design is binary then all diagonal elements of $L$ are equal to $r(k-1)$, and so

$$\hat{\theta}_1 + \cdots + \hat{\theta}_{v-1} = vr(k-1).$$

If these are all equal then their harmonic mean is

$$\frac{v(r(k-1))}{v-1}$$

and so

$$V_{\hat{\varepsilon}} = \hat{\varphi} = 2kr^2 \times \frac{v-1}{v(r(k-1))},$$

as we saw before for BIBDs.

If $\hat{\theta}_1, \ldots, \hat{\theta}_{v-1}$ are not all equal then their harmonic mean is smaller and so $\hat{\varphi}$ is larger.

### Optimal: Confidence region

When $v > 2$ the generalization of confidence interval is the confidence ellipsoid around the point $(\hat{\tau}_1, \ldots, \hat{\tau}_v)$ in the hyperplane in $\mathbb{R}^v$ with $\sum \hat{\tau}_i = 0$. The volume of this confidence ellipsoid is proportional to

$$\prod_{i=1}^{v-1} \frac{1}{\hat{\theta}_i} = \frac{\text{(geometric mean of } \hat{\theta}_1, \ldots, \hat{\theta}_{v-1})^{(v-1)/2}}{\sqrt{\text{number of spanning trees for } G}}$$

(Lecture II showed that the number of spanning trees for $G$ is

$$\hat{\theta}_1 \times \hat{\theta}_2 \times \cdots \times \hat{\theta}_{v-1},$$

using the notation $\lambda_1, \ldots, \lambda_v$ for $\hat{\theta}_1, \ldots, \hat{\theta}_v$)

### D-Optimality

A block design is called **D-optimal** if it minimizes the volume of the confidence ellipsoid around $(\hat{\varepsilon}_1, \ldots, \hat{\varepsilon}_v)$; 
—equivalently, it maximizes the geometric mean of the nontrivial eigenvalues of the Laplacian matrix $L$; 
—equivalently, it maximizes the number of spanning trees for the concurrence graph $G$; 
—equivalently, it maximizes the number of spanning trees for the Levi graph $\tilde{G}$, over all block designs with block size $k$ and the given $v$ and $b$.

### Optimality: Worst case

If $x$ is a contrast in $\mathbb{R}^v$ then the variance of the estimator of $x^\top \tau$ is $(x^\top L x)\lambda_{v-1}$.

If we multiply every entry in $x$ by a constant $c$ then this variance is multiplied by $c^2$, and $x^\top x$ is also multiplied by $c^2$.

The worst case is for contrasts $x$ giving the maximum value of $x^\top L x / x^\top x$.

These are precisely the eigenvectors corresponding to $\hat{\theta}_1$, where $\hat{\theta}_1$ is the smallest non-trivial eigenvalue of $L$.

### E-Optimality

A block design is called **E-optimal** if it maximizes the smallest non-trivial eigenvalue of the Laplacian matrix $L$, over all block designs with block size $k$ and the given $v$ and $b$. 
Section 7

Some optimal designs.

BIBDs are optimal

Theorem (Kshirsagar, 1958; Kiefer, 1975)
If there is a balanced incomplete-block design (BIBD) (2-design) for \( v \) treatments in \( b \) blocks of size \( k \), then it is \( A_\nu \), \( D \)- and \( E \)-optimal.

Proof
Let \( T = \text{Trace}(L) \). For any given value of \( T \), the harmonic mean of \( \theta_1, \ldots, \theta_{v-1} \), the geometric mean of \( \theta_1, \ldots, \theta_{v-1} \), and the minimum of \( \theta_1, \ldots, \theta_{v-1} \) are all maximized at \( T/(v-1) \) when \( \theta_1 = \cdots = \theta_{v-1} = T/(v-1) \). This occurs if and only if \( L \) is a scalar multiple of \( I - v^{-1} J \).

Since \( T = \sum (b\theta_i - \lambda_i) = b^2 - \sum \lambda_i \), the trace is maximized if and only if the design is binary. Among binary designs, the off-diagonal elements of \( L \) are equal if and only if the design is balanced.

Folklore about optimal designs

For many years after it was known that BIBDs are \( A_\nu \), \( D \)- and \( E \)-optimal, statisticians assumed the following:

- Only binary incomplete-block designs can be optimal.
- Optimal incomplete-block designs must have all their treatment replications as equal as possible.
- If an incomplete-block design is optimal on one of the three optimality criteria, then it must be optimal, or close to optimal, on the other two optimality criteria.

So we restricted our search for optimal designs, using these assumptions.

Now we know that all three assumptions are wrong.

Example 4: \( v = 5, b = 7, k = 3 \)

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<td>5</td>
<td>-2</td>
<td>-2</td>
<td>-2</td>
<td>8</td>
<td></td>
</tr>
</tbody>
</table>

maximal trace

1 2 3

eigenvalues equal

13, 10, 9

10, 10, 10, 10

harmonic mean

10.31

10

geometric mean

10.40

10

smallest

9

10

Some group-divisible optimal designs

Theorem (Cheng, 1981)
Group-divisible designs with two groups in which the between-group concurrence is one more than the within-group concurrence are \( A_\nu \), \( D \)- and \( E \)-optimal.

Theorem (Cheng, 1981)
Group-divisible designs in which the between-group concurrence is one more than the within-group concurrence are \( A_\nu \), \( D \)- and \( E \)-optimal among equireplicate designs whose concurrences differ by at most one.

### Some other optimal partially balanced designs

**Theorem (Cheng and Bailey, 1991)**

Partially balanced designs with two associate classes, in which the two concurrences differ by 1 and the matrix \((k) \cdot L = r \cdot C\) has an eigenvalue equal to 1 are A-, D- and E-optimal among binary equireplicate designs.

In particular, square-lattice designs are A-, D- and E-optimal among binary equireplicate designs.

**Comment**

Generalized quadrangles are a special case of partially balanced incomplete-block designs with two associate classes which satisfy these conditions.

### Section 8

Designs with very low replication.

The Levi graph has \(v+b\) vertices and \(bk\) edges.

For connectivity, \(bk \geq v+b-1\).

The extreme case is \(v-1 = b(k-1)\).

Then all connected Levi graphs are trees, so the D-criterion does not distinguish them.

In a tree, resistance distance is the same as graph distance, so the D-criterion does not distinguish them.

The Levi graph has \(v+b\) vertices and \(bk\) edges.

If it is connected and is not a tree then \(bk \geq v+b\).

The next case to consider is \(v-1 = b(k-1)\).

Then all connected Levi graphs are trees, so the D-criterion does not distinguish them.

The only E-optimal designs are the queen-bee designs.

### Lowest possible replication

The Levi graph has \(v+b\) vertices and \(bk\) edges.

For connectivity, \(bk \geq v+b-1\).

The extreme case is \(v-1 = b(k-1)\).

Then all connected Levi graphs are trees, so the D-criterion does not distinguish them.

In a tree, resistance distance is the same as graph distance, so the A-optimal designs have Levi graphs which are stars with a treatment-vertex at the centre.

These are just the queen-bee designs.

The E-optimal designs are also queen-bee designs.

### E-optimal designs when the Levi graph is a tree

By the Cutset Lemma, 
\[ \theta_1 \leq 2 \left( \frac{1}{5} + \frac{1}{10} \right) < 1 \]

This argument works for all non-queen-bee designs.

This argument works for all queen-bee designs.

The only E-optimal designs are the queen-bee designs.

### More details about the calculation for the queen-bee design

Label the treatments so that the queen-bee is 1. For the design shown in the previous slide with \(k = 3\), put treatments 2 and 3 in the same block, treatments 4 and 5 in the same block, and so on. Then the top left-hand corner of \(L\) is given by

\[
\begin{pmatrix}
14 & -1 & -1 & -1 & \ldots \\
-1 & 2 & -1 & 0 & 0 & \ldots \\
-1 & 0 & 0 & 2 & -1 & \ldots \\
-1 & 0 & 0 & -1 & 2 & \ldots \\
\vdots \\
\end{pmatrix}
\]

Put \(x = (0, 1, -1, 0, 0, \ldots, 0)^T\), \(y = (0, 1, 1, -1, 0, \ldots, 0)^T\) and \(z = (14, -1, -1, -1, \ldots, -1)^T\). Then \(Lx = 3x\) (in general, \(Lx = kx\)), \(Ly = y\); and \(Lz = 15z\) (in general, \(Lz = vz\)).

### Only slightly less extreme

The Levi graph has \(v+b\) vertices and \(bk\) edges.

If it is connected and is not a tree then \(bk \geq v+b\).

The next case to consider is \(v-1 = b(k-1)\).

Then every Levi graph has a single cycle.

The number of spanning trees for the Levi graph is equal to the length of the cycle, so the D-optimal designs have a cycle of length \(2b\). Like this…
Publications cited in these slides

A-optimal designs when the Levi graph has 1 cycle

Arguments using resistance in the Levi graph show that the A-optimal designs have a Levi graph with a short cycle, and one special treatment in the cycle occurs in every block which is not in the cycle.

A-optimal designs when the Levi graph has 1 cycle

For 2 ≤ s ≤ b, construct the design C(b, k, s) as follows.
▶ Construct a design for s treatments in s blocks of size 2 whose Levi graph is a single cycle.
▶ If k > 2, then insert k − 2 extra treatments into each block.
▶ If s < b, then designate one of the original s treatments as a "pseudo-queen".
▶ Each of the remaining b − s blocks contains the pseudo-queen and k − 1 further treatments.

Suppose that v = b(k − 1).

Some non-binary designs when the Levi graph has 1 cycle

Suppose that v = b(k − 1).

If k ≥ 3, then construct the design C(b, k, 1) as follows.
▶ Start with a single block of size 2 containing a single treatment twice.
▶ Insert k − 2 extra treatments into this block.
▶ If k > 3 then designate the treatment which occurs twice in this block as the queen-bee treatment.
▶ If k = 3 then either treatment in this block may be designated the queen-bee treatment.
▶ Each of the remaining b − 1 blocks contains the queen-bee treatment and k − 1 further treatments.

E-optimal designs when the Levi graph has 1 cycle

Suppose that v = b(k − 1).

If k ≥ 2 and v = bh ≥ 3 then the E-optimal designs are
▶ those in C(b, 2, b) if b ≤ 3;
▶ those in C(b, 2, 2) and those in C(b, 2, 1) if b ≥ 4.

Theorem
If k = 2 and v = bh ≥ 3 then the E-optimal designs are
▶ those in C(b, 2, b) if b ≤ 5;
▶ those in C(b, 2, 2), those in C(b, 2, 3) and those in C(b, 2, 2) if b = 6;
▶ those in C(b, 2, 3) and those in C(b, 2, 2) if b ≥ 7.

Best designs when the Levi graph has 1 cycle

Suppose that v = b(k − 1).

If 2 ≤ s ≤ b, construct the design C(b, k, s) as follows.
▶ Construct a design for s treatments in s blocks of size 2 whose Levi graph is a single cycle.
▶ If k > 2, then insert k − 2 extra treatments into each block.
▶ If s < b, then designate one of the original s treatments as a "pseudo-queen".
▶ Each of the remaining b − s blocks contains the pseudo-queen and k − 1 further treatments.

Main References