Laplacian eigenvalues and optimality: III. The Levi and concurrence graphs. Optimality

R. A. Bailey and Peter J. Cameron

Queen Mary University of London

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LTCC

Block designs

A block design Δ 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 ω.

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

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

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

Levi graph

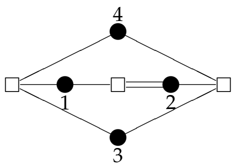
The Levi graph $\tilde{G}$ of a block design Δ has

- one vertex for each treatment,
- one vertex for each block,
- one edge for each experimental unit, with edge ω 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.

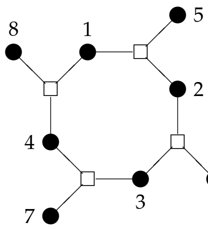
Example 1: $v = 4$, $b = k = 3$

1	2	1
3	3	2
4	4	2



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

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



Concurrence graph

The concurrence graph G of a block design Δ has

- one vertex for each treatment,
- one edge for each unordered pair α, ω, 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.

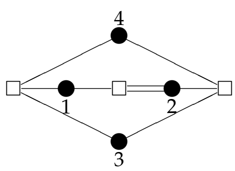
If $i \neq j$ then the number of edges between vertices i and j is

$$\lambda_{ij} = \sum_{s=1}^{b} N_{is} N_{js};$$

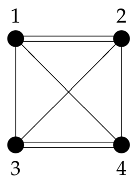
this is called the concurrence of i and j,
and is the (i,j)-entry of $\Lambda = NN^\top$.

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

1	2	1
3	3	2
4	4	2



Levi graph
can recover design
more vertices
more edges if $k = 2$

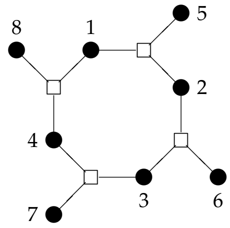


concurrence graph
may have more symmetry

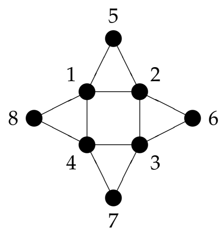
more edges if $k \geq 4$

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

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



Levi graph

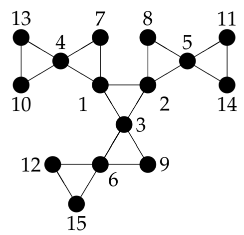


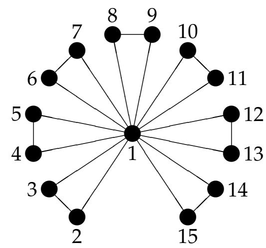
concurrence graph

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

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

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





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 $L_{ij} = -$(number of edges between i and j) $= -\lambda_{ij}$;
- $L_{ii} =$ valency of $i = \sum_{j \neq i} \lambda_{ij}$.

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:

- $\tilde{L}_{ii} =$ valency of i
$$= \begin{cases} k & \text{if } i \text{ is a block} \\ \text{replication } r_i \text{ of } i & \text{if } i \text{ is a treatment} \end{cases}$$
- if $i \neq j$ then $L_{ij} = -$(number of edges between i and j)
$$= \begin{cases} 0 & \text{if } i \text{ and } j \text{ are both treatments} \\ 0 & \text{if } i \text{ and } j \text{ are both blocks} \\ -N_{ij} & \text{if } i \text{ is a treatment and } j \text{ is a block, or vice versa.} \end{cases}$$

$$\text{So} \quad \tilde{L} = \begin{bmatrix} R & -N \\ -N^\top & kI_b \end{bmatrix},$$

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. *0 is a simple eigenvalue of L;*
2. *G is a connected graph;*
3. *$\tilde{G}$ is a connected graph;*
4. *0 is a simple eigenvalue of $\tilde{L}$;*
5. *the design Δ 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.

Variance: why does it matter?

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

Put $V_{ij} =$ 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, then 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 τ_1 and τ_2 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 σ^2.
If $\sum_i x_i = 0$, then the variance of the best linear unbiased estimator of $\sum_i x_i \tau_i$ is equal to

$$(x^\top L^- x)k\sigma^2.$$

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

$$V_{ij} = \left(L^-_{ii} + L^-_{jj} - 2L^-_{ij}\right) k\sigma^2.$$

... 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

$$V_{ij} = \left(\tilde{L}^-_{ii} + \tilde{L}^-_{jj} - 2\tilde{L}^-_{ij}\right) \sigma^2.$$

Electrical networks: variance and resistance

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

Theorem
The effective resistance R_{ij} between vertices i and j in G is

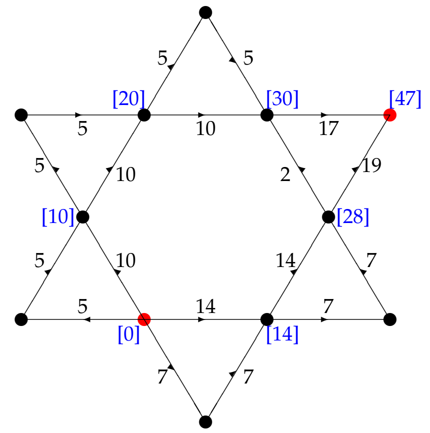
$$R_{ij} = \left(L^-_{ii} + L^-_{jj} - 2L^-_{ij}\right).$$

So

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

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

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



$V = 47$

$I = 36$

$R = \dfrac{47}{36}$

... Or we can use the Levi graph

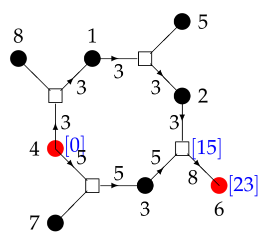
If i and j are treatment vertices in the Levi graph $\tilde{G}$ and $\tilde{R}_{ij}$ is the effective resistance between them in $\tilde{G}$ then

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

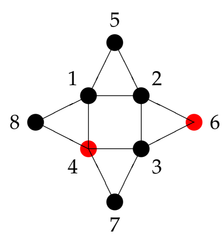
Example 2 yet again: $v = 8$, $b = 4$, $k = 3$

$V = 23 \quad I = 8 \quad R = \dfrac{23}{8}$

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



Levi graph



concurrence graph

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 $k \geq 3$.

Spanning trees in the two graphs

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

$$t = \det L_1 = \det(kR_1 - N_1 N_1^\top) \quad \text{and} \quad \tilde{t} = \det \tilde{L}_1,$$

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

$$\begin{aligned}\det \tilde{L}_1 &= \det \begin{bmatrix} R_1 & -N_1 \\ -N_1^\top & kI_b \end{bmatrix} = \det \begin{bmatrix} R_1 - k^{-1}(N_1)N_1^\top & -N_1 \\ -N_1^\top + k^{-1}(kI_b)N_1^\top & kI_b \end{bmatrix} \\ &= \det \begin{bmatrix} k^{-1}L_1 & -N_1 \\ 0 & kI_b \end{bmatrix} = k^{-(v-1)} \det L_1 \times k^b\end{aligned}$$

$$\text{so} \quad \tilde{t} = \det \tilde{L}_1 = k^{b-v+1} \det L_1 = k^{b-v+1} t.$$

□

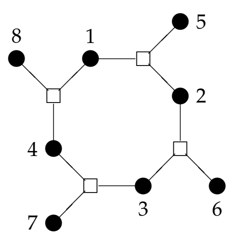
Spanning trees in the two graphs: strategy

If $v \geq b+2$ then count the number of spanning trees for the Levi graph, then multiply by k^{v-b-1} to obtain the number of spanning trees for the concurrence graph.

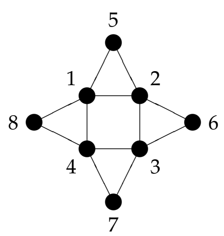
If $v \leq b$ then do it the other way round.

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

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



Levi graph
8 spanning trees



concurrence graph
216 spanning trees

Optimality: Average pairwise variance

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

$$V_{ij} = \left(L^-_{ii} + L^-_{jj} - 2L^-_{ij}\right) k\sigma^2 = R_{ij} k \sigma^2.$$

We want all of the V_{ij} to be small.

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

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

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

A-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 non-trivial eigenvalues of the Laplacian matrix L;
over all block designs with block size k and the given v and b.

Optimality: 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 $\sum_i \tau_i = 0$. The volume of this confidence ellipsoid is proportional to

$$\sqrt{\prod_{i=1}^{v-1} \frac{1}{\theta_i}} = (\text{geometric mean of } \theta_1, \ldots, \theta_{v-1})^{-(v-1)/2}$$
$$= \frac{1}{\sqrt{v \times \text{number of spanning trees for } G}}.$$

D-Optimality

A block design is called D-optimal if it minimizes the volume of the confidence ellipsoid for $(\hat{\tau}_1, \ldots, \hat{\tau}_v)$;
—equivalently, it maximizes the geometric mean of the non-trivial 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 $(x^\top L^- x)k\sigma^2$.

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

The worst case is for contrasts x giving the maximum value of

$$\frac{x^\top L^- x}{x^\top x}.$$

These are precisely the eigenvectors corresponding to θ_1, where θ_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.

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-, D- and E-optimal.
Moreover, no non-BIBD is A-, D- or E-optimal.*

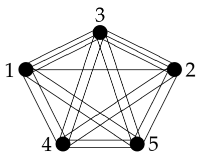
Proof.
Let $T = \mathrm{Trace}(L)$. For any given value of T, the harmonic mean of $\theta_1, \ldots, \theta_{v-1}$, the geometric mean of $\theta_1, \ldots, \theta_{v-1}$, and the minimum of $\theta_1, \ldots, \theta_{v-1}$ are all maximized at $T/(v-1)$ when $\theta_1 = \cdots = \theta_{v-1} = T/(v-1)$. This occurs if and only if L is a scalar multiple of $I_v - v^{-1}J_v$.
Since $T = \sum_i (kr_i - \lambda_{ii}) = bk^2 - \sum_i \lambda_{ii}$, 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. □

Example 4: $v = 5$, $b = 7$, $k = 3$

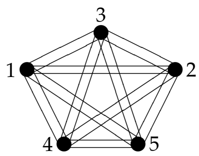
1	1	1	1	2	2	2
2	3	3	4	3	3	4
3	4	5	5	4	5	5

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

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



maximal trace



eigenvalues equal

Some other classes of optimal design

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-, 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-, D- and E-optimal among equireplicate designs whose concurrences differ by at most one.

Theorem (Cheng and Bailey, 1991)

Square-lattice designs are A-, D- and E-optimal among binary equireplicate designs.

Very low replication

The Levi graph has $v + b$ vertices and bk edges.

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

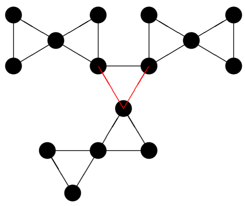
The extreme case is $v - 1 = b(k - 1)$.

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

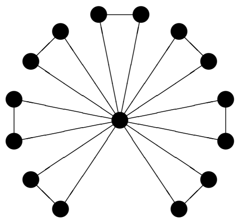
In a tree, pairwise resistance is just distance apart,
so the A-optimal designs have Levi graphs which are stars
with a treatment-vertex at the centre:
these are just the queen-bee designs.

The E-optimal designs are also queen-bee designs:
proof coming up.

E-optimal designs when the Levi graph is a tree



$$\theta_1 \leq 2\left(\frac{1}{5} + \frac{1}{10}\right) < 1$$



eigenvalues 1 (between block),
k (within block), v (queen vs rest)

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

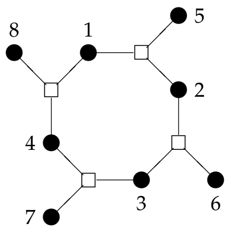
Only slightly less extreme

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 $v = b(k - 1)$.

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 . . .



A- and E-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.

Arguments using the Cutset Lemma in the concurrence graph show that the E-optimal designs have similar structure, usually with an even shorter cycle in the Levi graph.