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

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Groups and Graphs, Designs and Dynamics
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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.

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

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

Outline

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

Section 1

Two graphs associated with a block design.

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Some other authors call it the incidence graph.

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3	3	2
4	4	2

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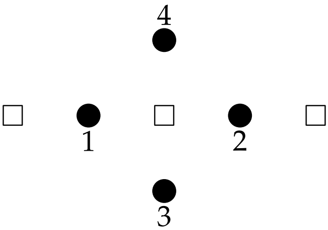

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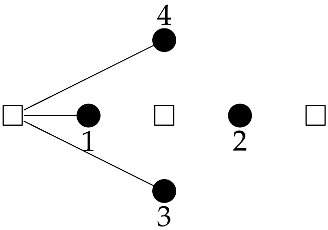

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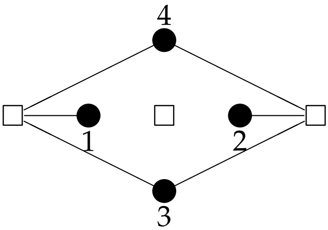

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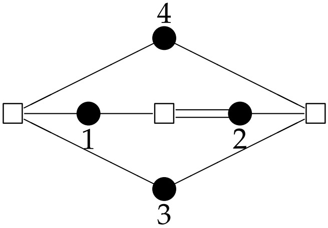

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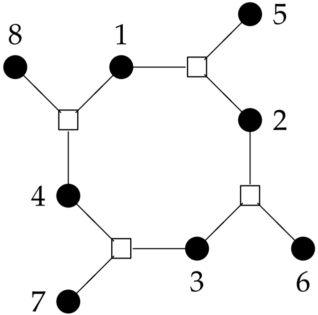

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If $i \neq j$ then the number of edges between vertices i and j is

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

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

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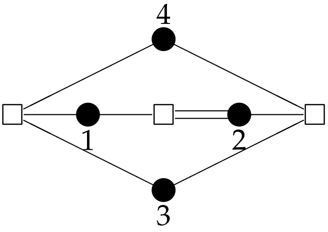

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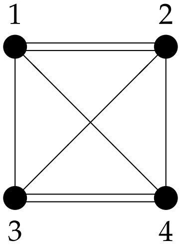

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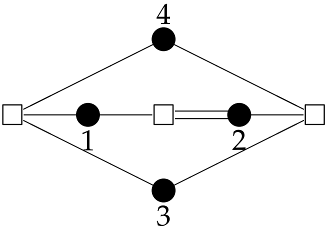
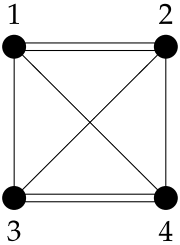


Levi graph
can recover design



concurrence graph
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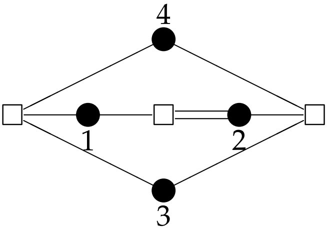

Levi graph
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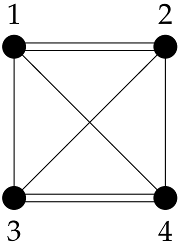
more vertices



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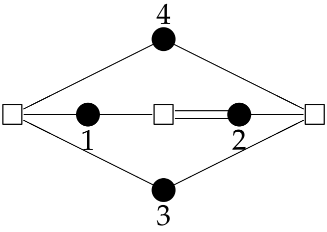

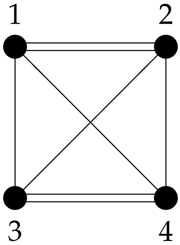

Levi graph
can recover design
more vertices
more edges if $k = 2$

concurrence graph
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more edges if $k \geq 4$

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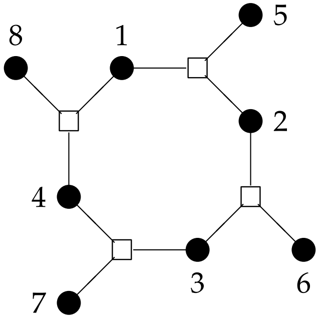

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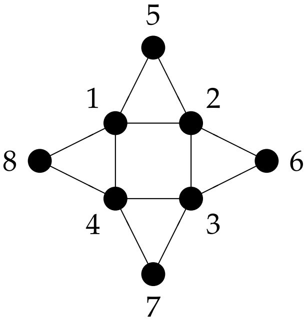

concurrence graph

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

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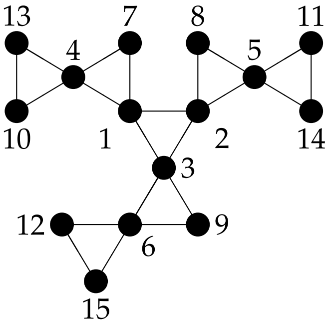

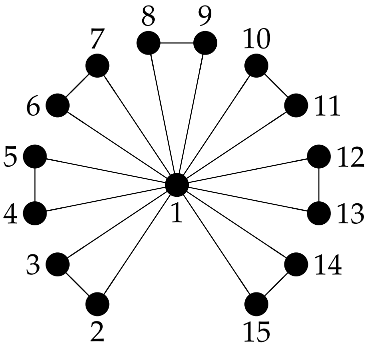

Section 2

Laplacian matrices.

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

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

$$= \begin{cases} 0 & \text{if } i \text{ and } j \text{ are both treatments} \\ 0 & \text{if } i \text{ and } j \text{ are both blocks} \\ -N_{ij} & \text{if } i \text{ is a treatment and } j \text{ is a block, or vice versa.} \end{cases}$$

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

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

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

Section 3

Estimation and variance.

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 $\sqrt{V_{ij}}$.

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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

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

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Comment

All vectors in this lecture are column vectors.

. . . Or we can use the Levi graph

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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.

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

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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 $[x]$.

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

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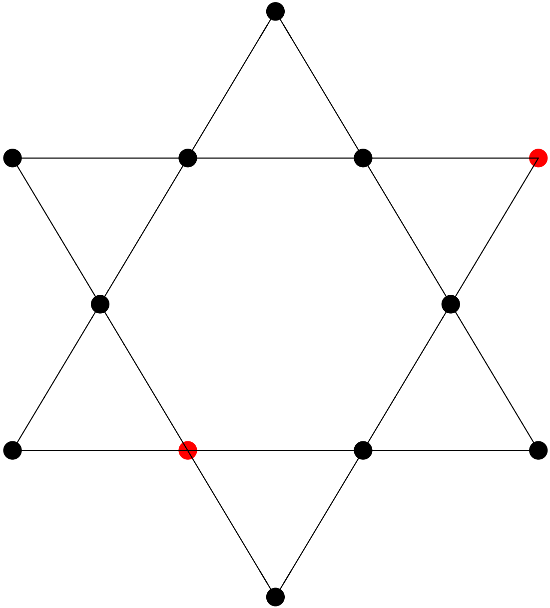
Ohm's Law gives

$$V = IR,$$

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

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



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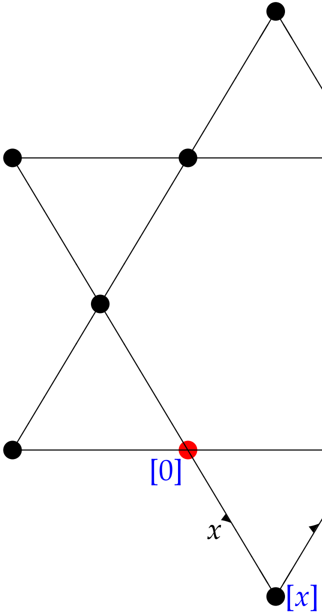

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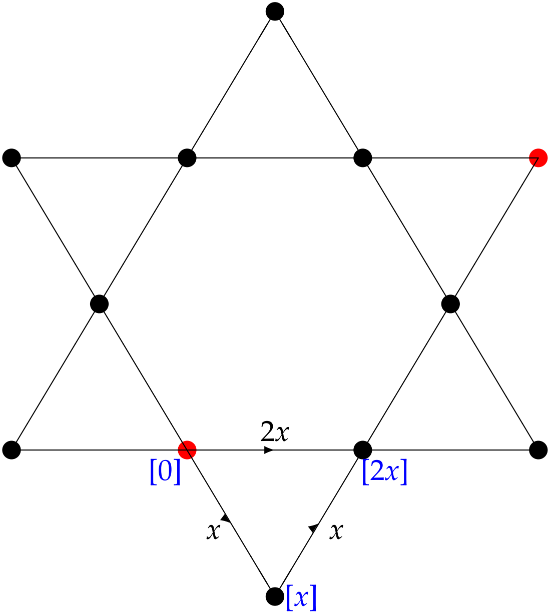

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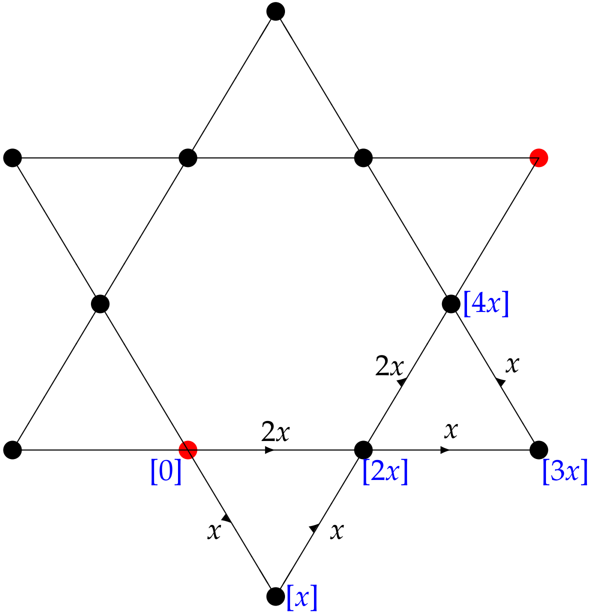

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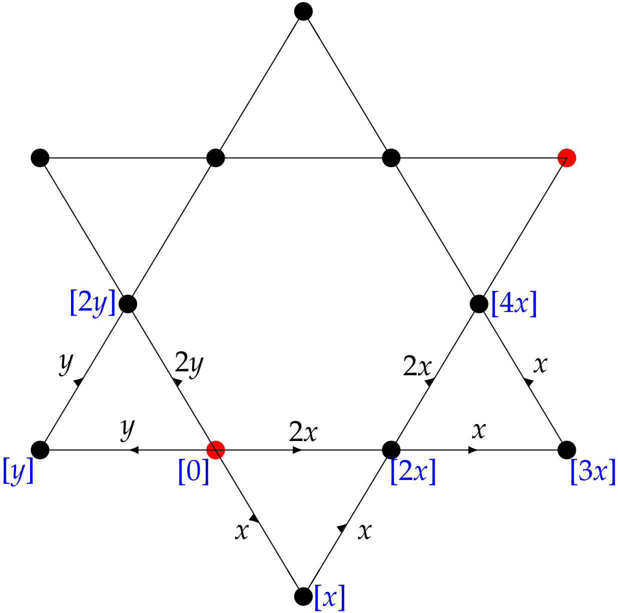

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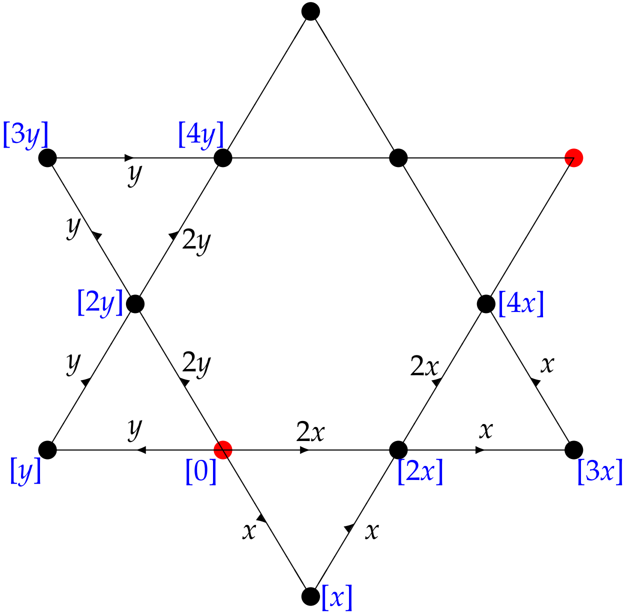

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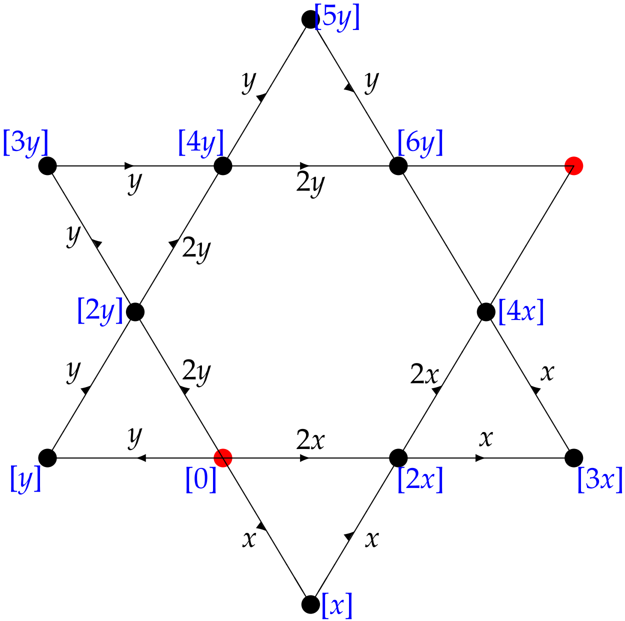

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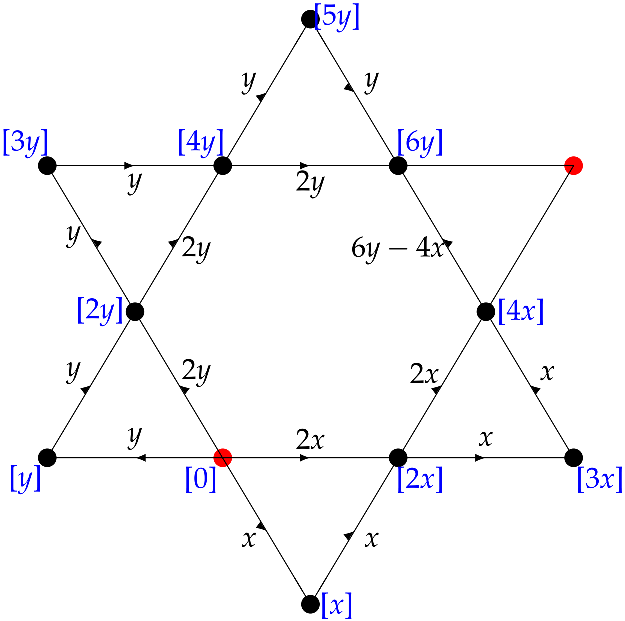

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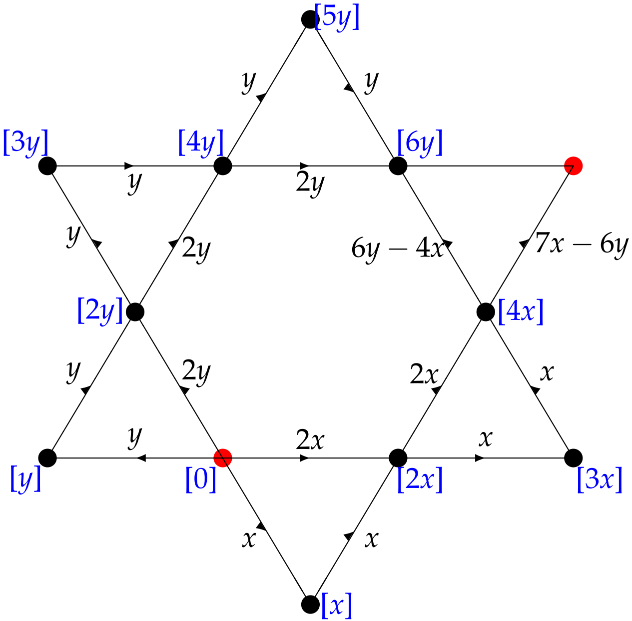

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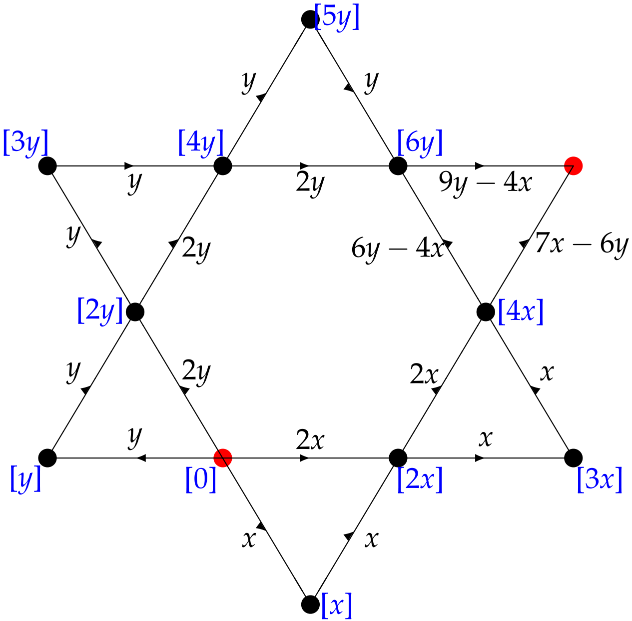

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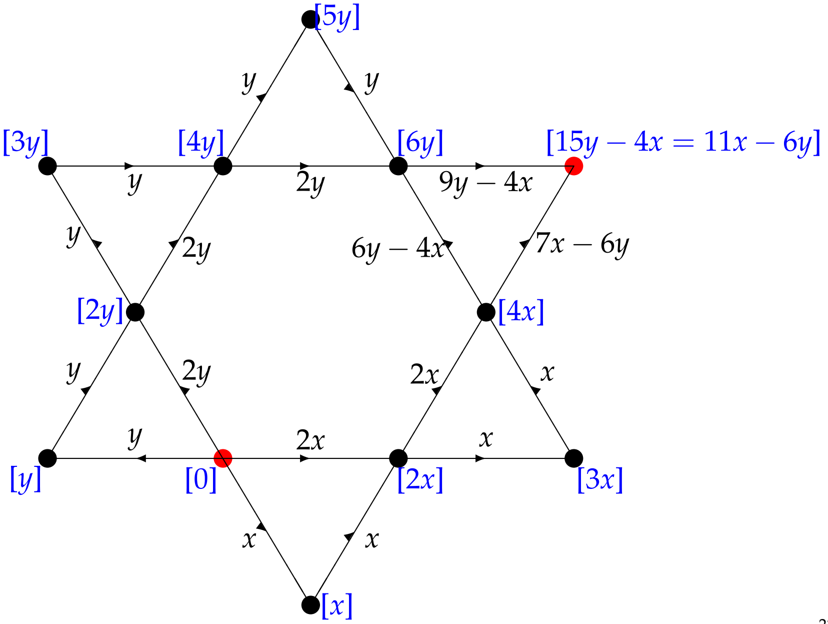

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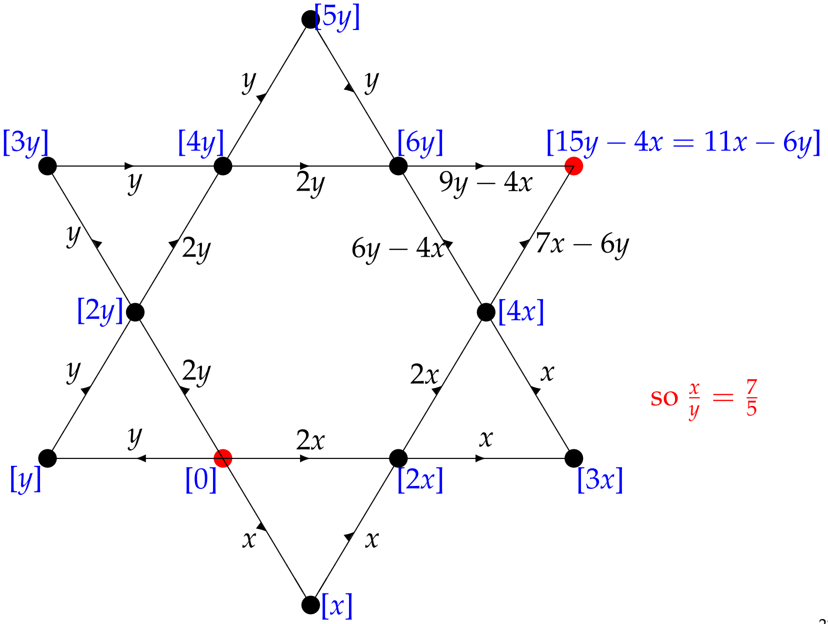

so $\frac{x}{y} = \frac{7}{5}$

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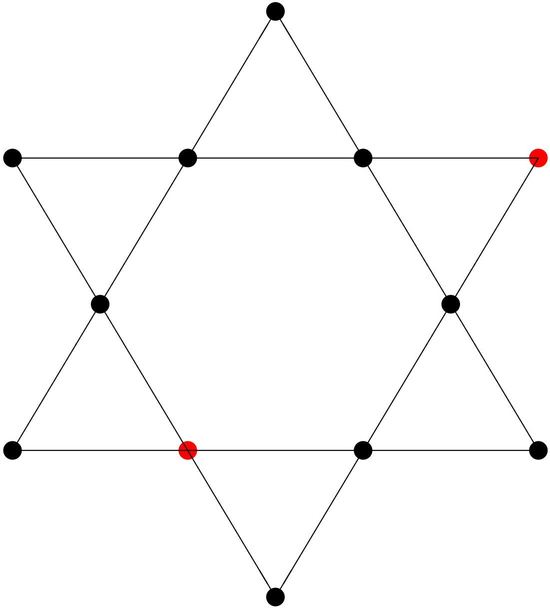

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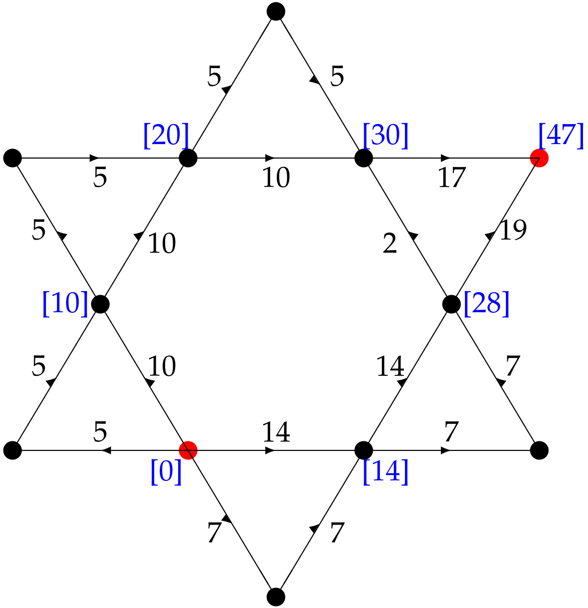

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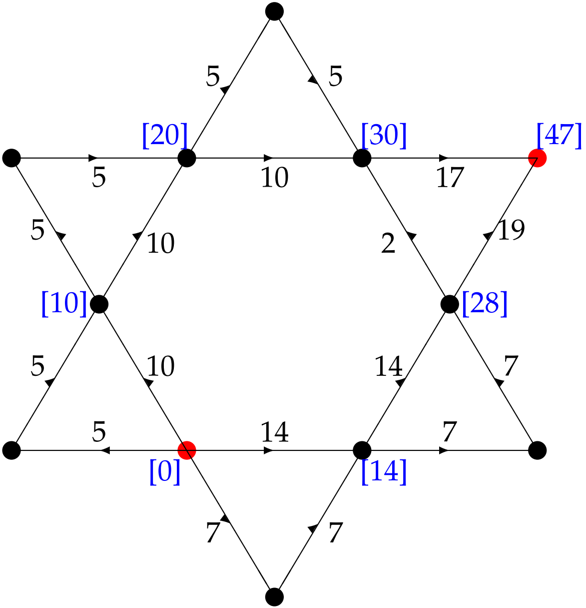


$V = 47$

$I = 36$

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

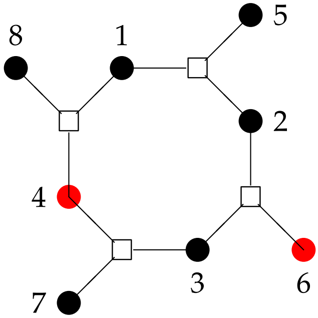
. . . Or we can use the Levi graph

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

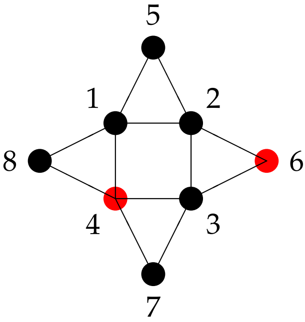
$$V_{ij} = \tilde{R}_{ij} \times \sigma^2.$$

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

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



Levi graph



concurrence graph

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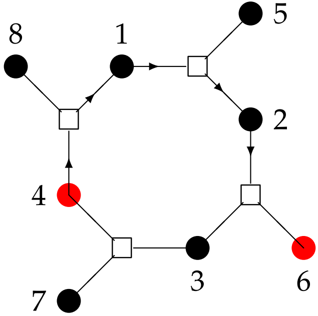

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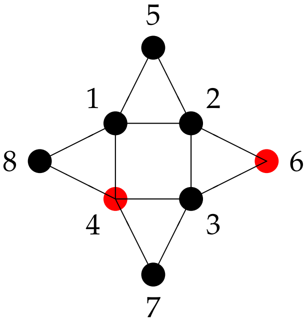

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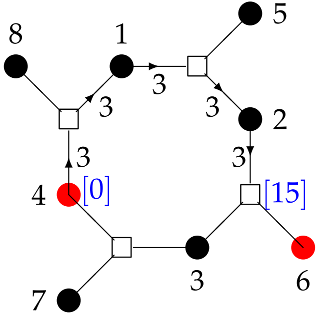

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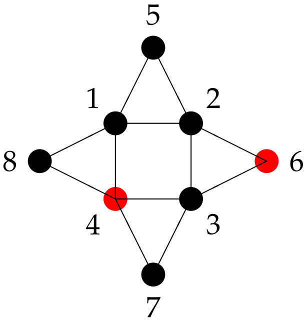

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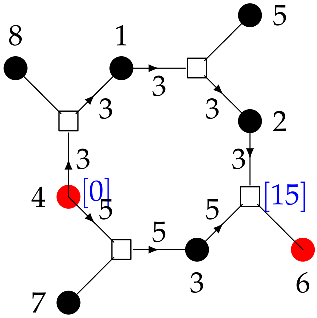

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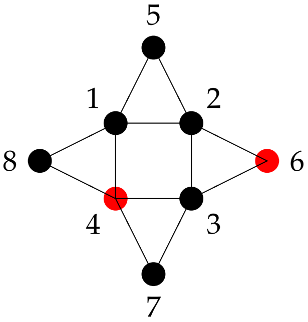

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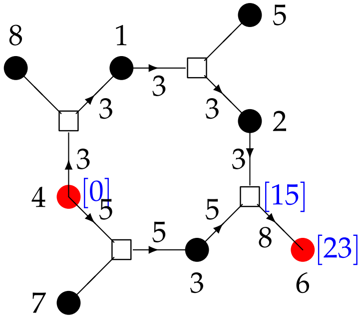

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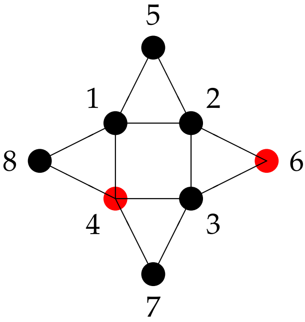

concurrence graph

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

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

1	2	3	4
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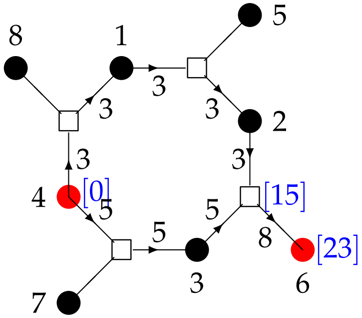
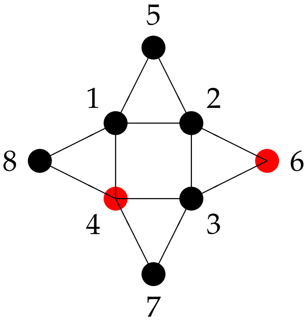
5	6	7	8

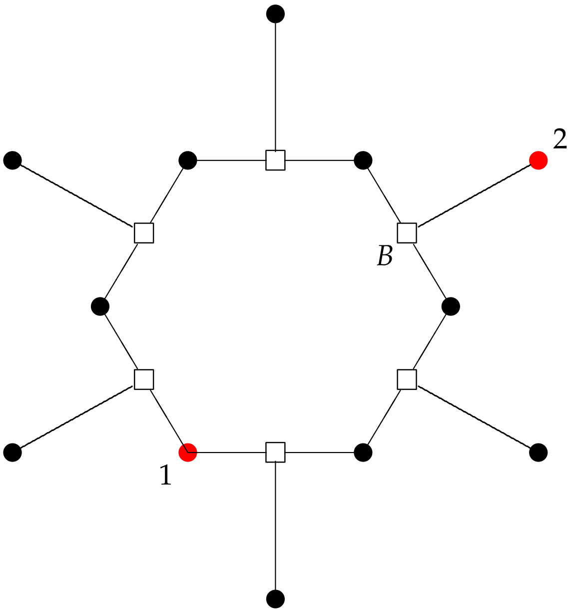


Levi graph



concurrence graph

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.

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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

$$\tilde{R}_{1B} = \frac{1}{\frac{1}{5} + \frac{1}{7}} = \frac{1}{\frac{12}{35}} = \frac{35}{12}.$$

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$$\tilde{R}_{1B} = \frac{1}{\frac{1}{5} + \frac{1}{7}} = \frac{1}{\frac{12}{35}} = \frac{35}{12}.$$

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.

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

$$t = \det L_1 \qquad \text{and} \qquad \tilde{t} = \det \tilde{L}_1,$$

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

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$$\det \tilde{L}_1 = \det \begin{bmatrix} R_1 & -N_1 \\ -N_1^\top & kI_b \end{bmatrix}$$

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

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.

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

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&= \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}$$

Spanning trees in the two graphs: proof

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

□

Spanning trees in the two graphs: strategy

We have shown that

$$\tilde{t} = k^{b-v+1}t,$$

where t is the number of spanning trees for the concurrence graph and $\tilde{t}$ is the number of spanning trees for the Levi graph.

Spanning trees in the two graphs: strategy

We have shown that

$$\tilde{t} = k^{b-v+1}t,$$

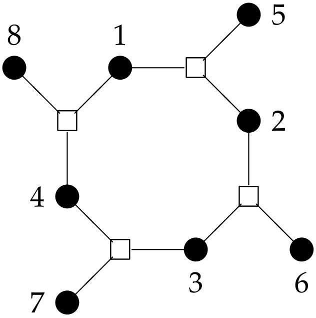
where t is the number of spanning trees for the concurrence graph and $\tilde{t}$ is the number of spanning trees for the Levi graph.

If $v \geq b+2$ then $\tilde{t} < t$, so 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.

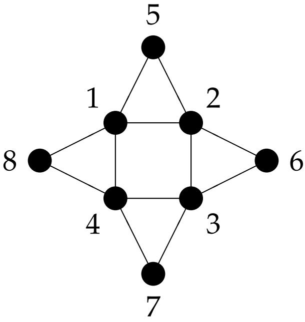
If $v \leq b$ then do it the other way round.

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

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



Levi graph



concurrence graph

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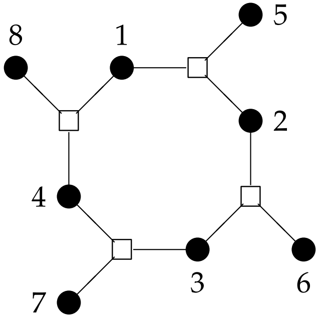
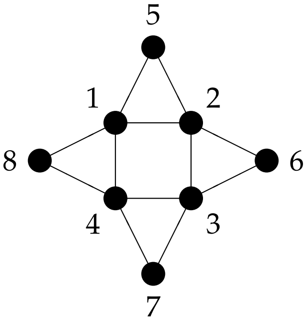


Levi graph
8 spanning trees



concurrence graph

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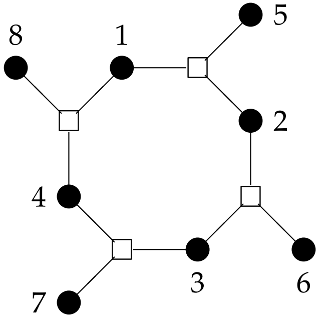

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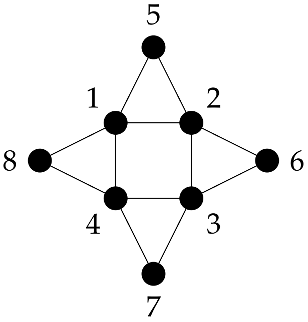

concurrence graph
216 spanning trees

Section 6

Measures of optimality.

Optimality: Average pairwise variance

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

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

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

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

$$\frac{1}{k\sigma^2}\sum_{1\le i<j\le v} V_{ij} \quad = \quad (v-1)\sum_i L^-_{ii} - \sum_{i\neq j} L^-_{ij}$$

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&= v \sum_i L^-_{ii} \quad \text{because the row sums of } L^- \text{ are zero} \\
&= v \,\text{Trace}(L^-)
\end{aligned}$$

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

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

$$\begin{aligned}
\frac{1}{k\sigma^2}\sum_{1\le i<j\le v} V_{ij} &= (v-1)\sum_i L^-_{ii} - \sum_{i\neq j} L^-_{ij} \\
&= v\sum_i L^-_{ii} \quad \text{because the row sums of } L^- \text{ are zero} \\
&= v\,\mathrm{Trace}(L^-) \\
&= v\left(\frac{1}{\theta_1} + \cdots + \frac{1}{\theta_{v-1}}\right),
\end{aligned}$$

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

Optimality: Average pairwise variance, continued

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$$= 2k\sigma^2 \times \frac{1}{\text{harmonic mean of } \theta_1, \ldots, \theta_{v-1}},$$

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as we saw before for BIBDs.

If $\theta_1 \ldots, \theta_{v-1}$ are not all equal then
their harmonic mean is smaller and so $\bar{V}$ is larger.

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

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

$$\frac{\theta_1 \times \theta_2 \times \cdots \times \theta_{v-1}}{v},$$

using the notation $\lambda_2, \ldots, \lambda_n$ for $\theta_1, \ldots, \theta_v$.)

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These are precisely the eigenvectors corresponding to θ_1, where θ_1 is the smallest non-trivial eigenvalue of L.

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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-, D- and E-optimal. Moreover, in this case, no non-BIBD is A-, D- or E-optimal.

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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 $I_v - v^{-1}J_v$.

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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. □

Folklore about optimal designs

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

Now we know that all three assumptions are wrong.

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

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

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

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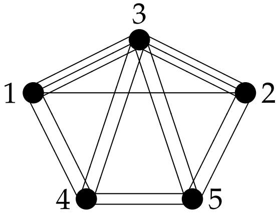

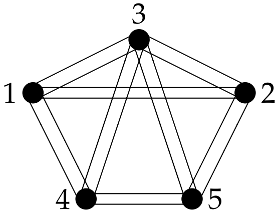

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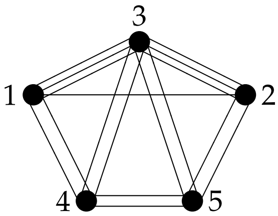

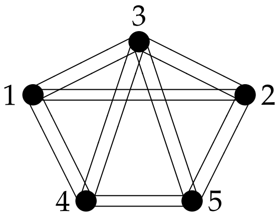

eigenvalues equal

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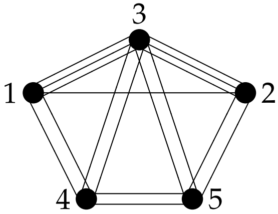

maximal trace

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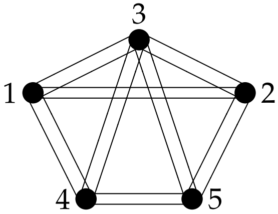

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	maximal trace	eigenvalues equal
eigenvalues	13, 10, 10, 9	10, 10, 10, 10

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	maximal trace	eigenvalues equal
eigenvalues	13, 10, 10, 9	10, 10, 10, 10
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geometric mean	10.40	10
smallest	9	10

Some group-divisible optimal designs

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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.

Some other optimal partially balanced designs

Theorem (Cheng and Bailey, 1991)

Partially balanced designs with two associate classes,
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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.

Lowest possible replication

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these are just the queen-bee designs.

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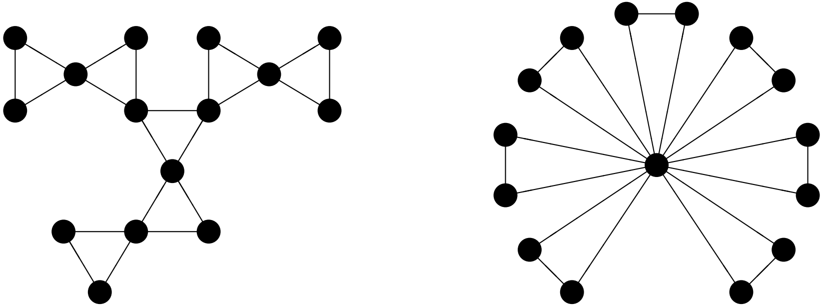
The E-optimal designs are also queen-bee designs:
proof coming up.

E-optimal designs when the Levi graph is a tree



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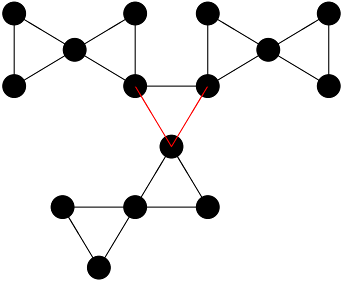

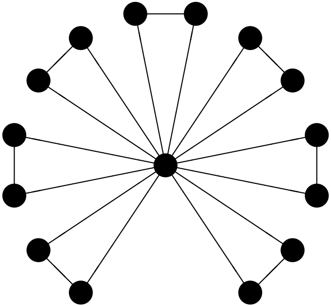

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$$\theta_1 \leq 2\left(\frac{1}{5} + \frac{1}{10}\right) < 1$$

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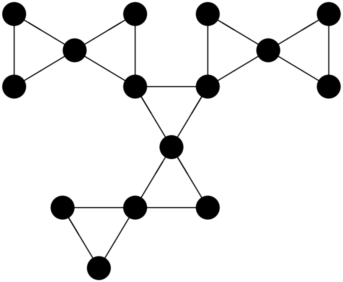

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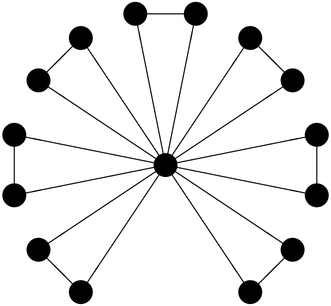
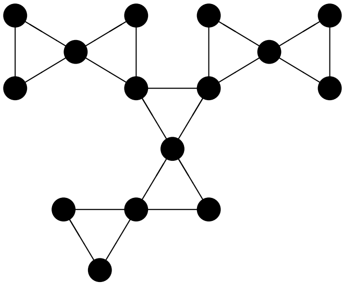


eigenvalues 1 (between blocks),

k (within any block), v (queen vs rest)

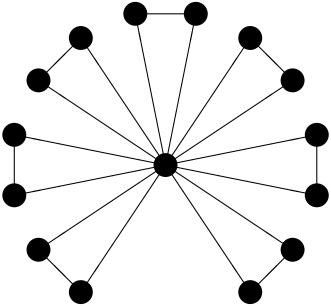
E-optimal designs when the Levi graph is a tree



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



eigenvalues 1 (between blocks),

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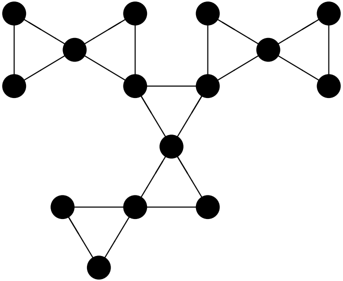

By the Cutset Lemma,

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

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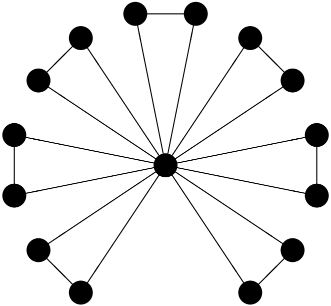

eigenvalues 1 (between blocks), k (within any block), v (queen vs rest)

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

$$\begin{bmatrix} 14 & -1 & -1 & -1 & -1 & \dots \\ -1 & 2 & -1 & 0 & 0 & \dots \\ -1 & -1 & 2 & 0 & 0 & \dots \\ -1 & 0 & 0 & 2 & -1 & \dots \\ -1 & 0 & 0 & -1 & 2 & \dots \\ \vdots & & & & & \end{bmatrix}$$

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Put $x = (0, 1, -1, 0, 0, \ldots, 0)^\top$, $y = (0, 1, 1, -1, -1, 0, \ldots, 0)^\top$ and $z = (14, -1, -1, -1, -1, \ldots, -1)^\top$.

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

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

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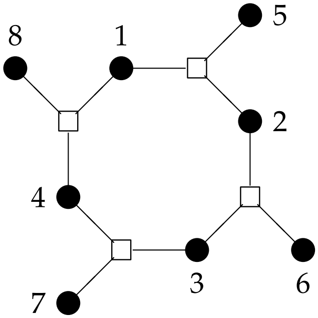

A- and E-optimal designs when the Levi graph has 1 cycle

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.

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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.

Best designs when the Levi graph has 1 cycle

Suppose that $v = b(k-1)$.

For $2 \leq s \leq b$, construct the design $\mathcal{C}(b,k,s)$ as follows.

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- Each of the remaining $b-s$ blocks contains the pseudo-queen and $k-1$ further treatments.

A-optimal designs when the Levi graph has 1 cycle

Theorem

If $v = b(k-1)$ then the A-optimal designs are those in $\mathcal{C}(b,k,s)$, where the value of s is given in the following table.

k \ b	2	3	4	5	6	7	8	9	10	11	12	≥ 13
2	2	3	4	5	6	7	8	4	4	4	3 *or* 4	3
3	2	3	4	5	6	3	3	3	3	3	2	2
4	2	3	4	5	3	2	2	2	2	2	2	2
5	2	3	4	5	2	2	2	2	2	2	2	2
≥ 6	2	3	4	2	2	2	2	2	2	2	2	2

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

Suppose that $v = b(k-1)$.

If $k \geq 3$, then construct the design $\mathcal{C}(b,k,1)$ as follows.

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

Suppose that $v = b(k-1)$.

If $k \geq 3$, then construct the design $\mathcal{C}(b, k, 1)$ as follows.

- Start with a single block of size 2 containing a single treatment twice.

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Suppose that $v = b(k-1)$.

If $k \geq 3$, then construct the design $\mathcal{C}(b, k, 1)$ as follows.

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- 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.

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  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

Theorem

If $v = b(k-1)$ *and* $b \geq 3$ *and* $k \geq 3$ *then the E-optimal designs are*

- *those in* $\mathcal{C}(b,k,b)$ *if* $3 \leq b \leq 4$*;*
- *those in* $\mathcal{C}(b,k,2)$ *and those in* $\mathcal{C}(b,k,1)$ *if* $b \geq 5$*.*

E-optimal designs when the Levi graph has 1 cycle

Theorem

If $v = b(k-1)$ and $b \geq 3$ and $k \geq 3$ then the E-optimal designs are

- *those in $\mathcal{C}(b,k,b)$ if $3 \leq b \leq 4$;*
- *those in $\mathcal{C}(b,k,2)$ and those in $\mathcal{C}(b,k,1)$ if $b \geq 5$.*

Theorem

If $k = 2$ and $v = b \geq 3$ then the E-optimal designs are

- *those in $\mathcal{C}(b,2,b)$ if $b \leq 5$;*
- *those in $\mathcal{C}(b,2,b)$, those in $\mathcal{C}(b,2,3)$ and those in $\mathcal{C}(b,2,2)$ if $b = 6$;*
- *those in $\mathcal{C}(b,2,3)$ and those in $\mathcal{C}(b,2,2)$ if $b \geq 7$.*

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