Levi graphs and concurrence graphs as tools to evaluate block designs

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(Joint work with Peter J. Cameron)

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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.

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The treatments are the 16 new detergents.

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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.

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

binary

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

non-binary

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

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

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

replications differ by ≤ 1

1	1	1	1	1	1	1
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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?

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

balanced (2-design)

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

non-balanced

A binary design is balanced if every pair of distinct treaments occurs together in the same number of blocks.

Experimental units and incidence matrix

There are bk experimental units.

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

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The $v \times b$ incidence matrix N has entries n_{ij}.

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

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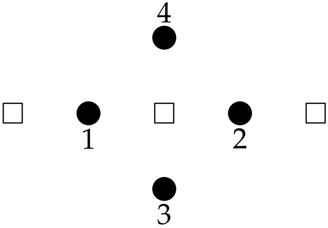

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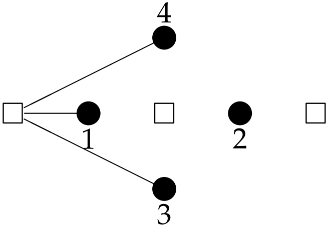

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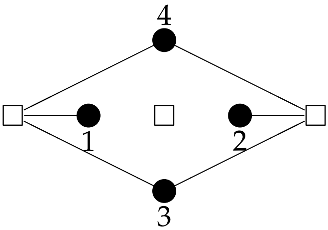

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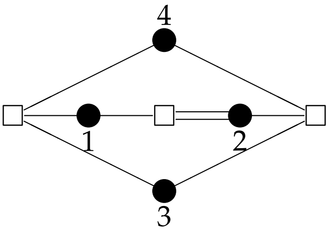

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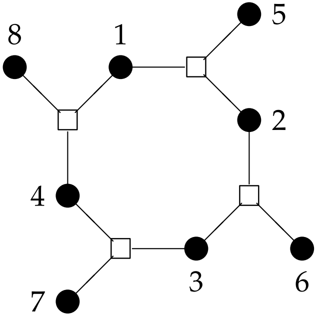

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$$\lambda_{ij} = \sum_{s=1}^{b} n_{is} n_{js};$$

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

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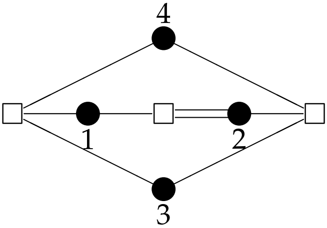

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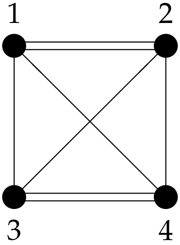

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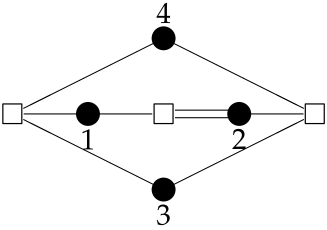
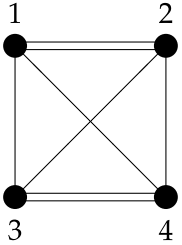


Levi graph
can recover design



concurrence graph
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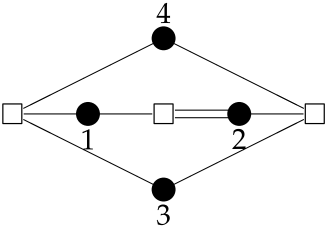

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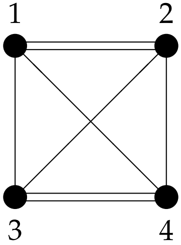

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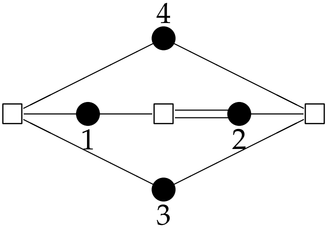
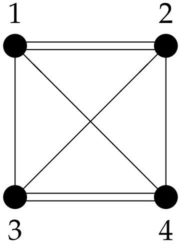


Levi graph
can recover design
more vertices
more edges if $k = 2$



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more edges if $k \geq 4$

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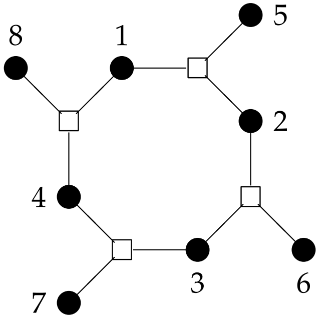

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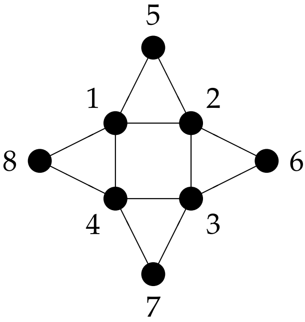

concurrence graph

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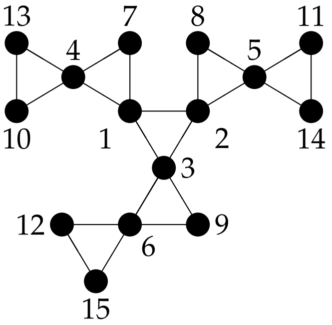

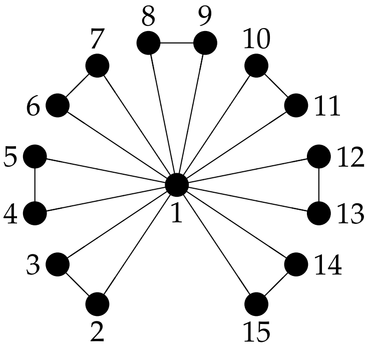

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- $\tilde{L}_{ii} =$ valency of i

$$= \begin{cases} k & \text{if } i \text{ is a block} \\ \text{replication } r_i \text{ of } i & \text{if } i \text{ is a treatment} \end{cases}$$

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

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

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The following are equivalent.

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2. G *is a connected graph;*
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Call the remaining eigenvalues *non-trivial*.
They are all non-negative.

Under the assumption of connectivity,
the Moore–Penrose generalized inverse L^- of L is defined by

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

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The Moore–Penrose generalized inverse $\tilde{L}^-$ of $\tilde{L}$ is defined similarly.

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

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 $\tau_i - \tau_j$.

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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

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How do we calculate variance?

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Electrical networks

We can consider the concurrence graph G as an electrical network with a 1-ohm resistance in each edge.
Connect a 1-volt battery between vertices i and j.
Current flows in the network, according to these rules.

1. Ohm's Law:
   In every edge, voltage drop = current $\times$ resistance = 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 $1/I$.

Electrical networks: variance

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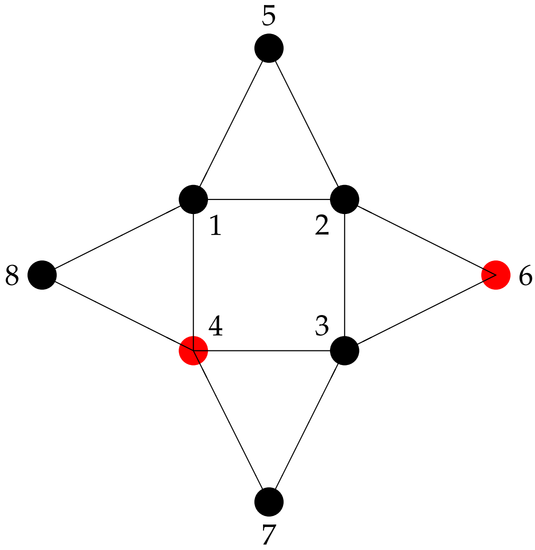
Effective resistances are easy to calculate without matrix inversion if the graph is sparse.

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



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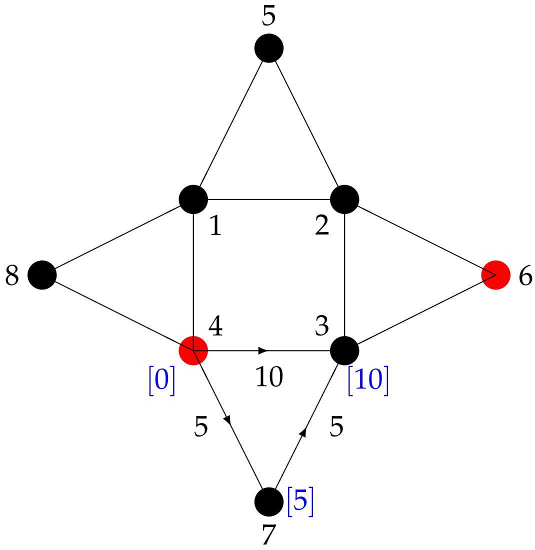

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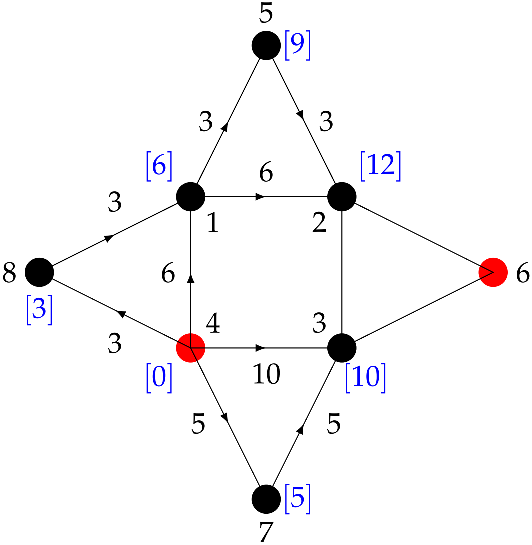

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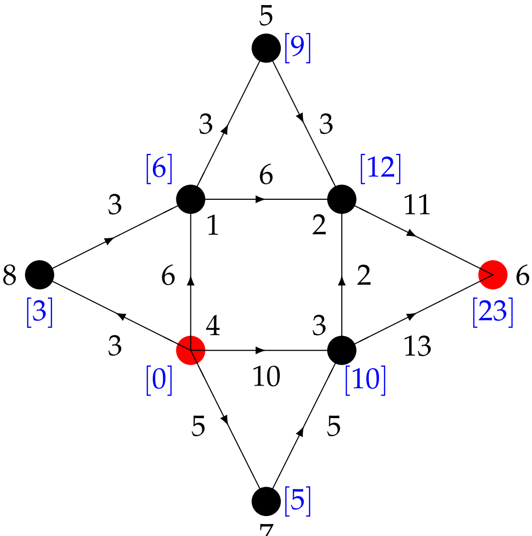
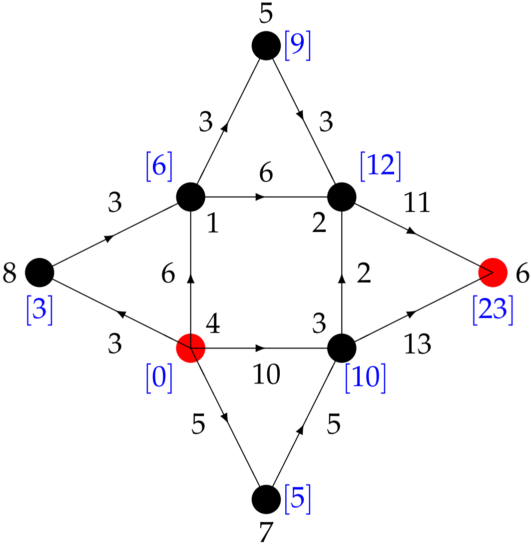


Example 2 calculation: $v = 8$, $b = 4$, $k = 3$

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



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

1	2	3	4
2	3	4	1
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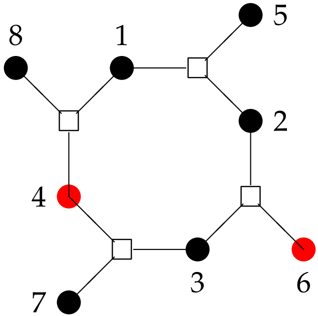

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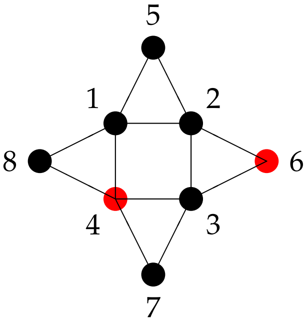

concurrence graph

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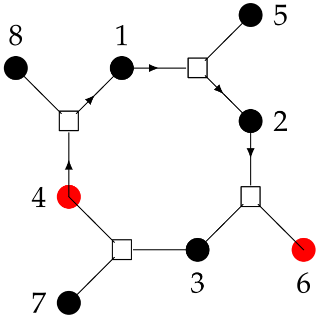

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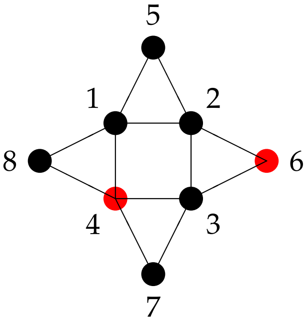

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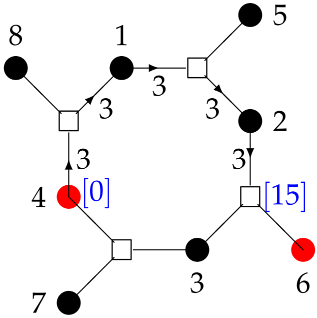

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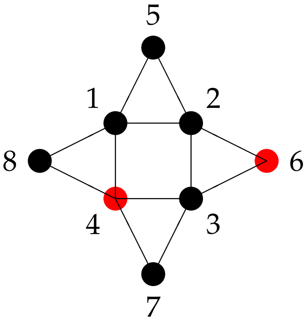

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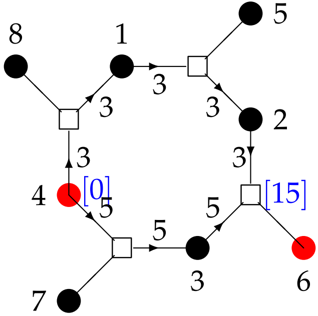

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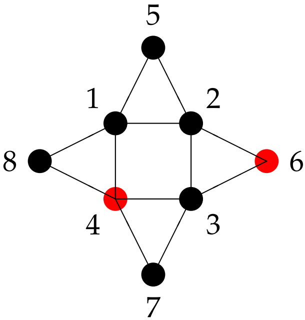

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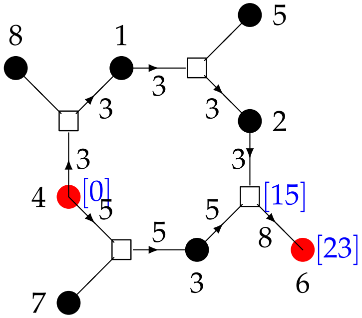

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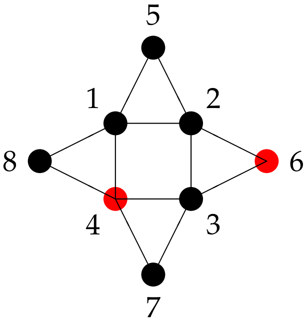

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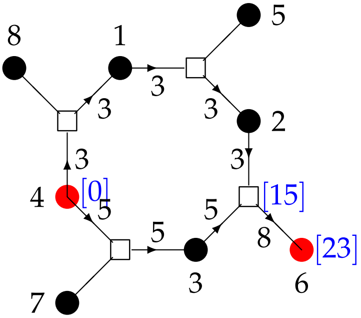

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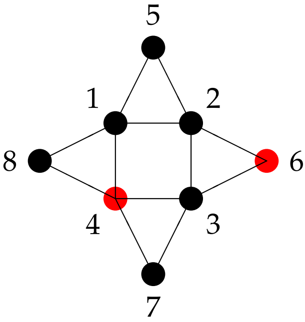

concurrence graph

Optimality: Average pairwise variance

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.

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.

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

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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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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.

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.

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Cheng (1981), after Gaffke (1978), after Kirchhoff (1847):

$$\begin{aligned} & \text{product of non-trivial eigenvalues of } L \\ = \quad & v \times \text{number of spanning trees.} \end{aligned}$$

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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.

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 $\tilde{G}$ is equal to k^{b-v+1} times the number of spanning trees for G.

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

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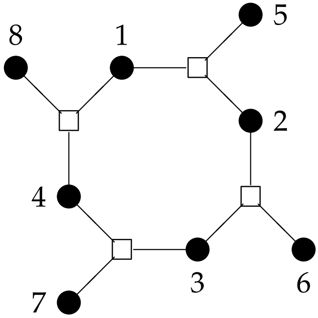
2	3	4	1
5	6	7	8



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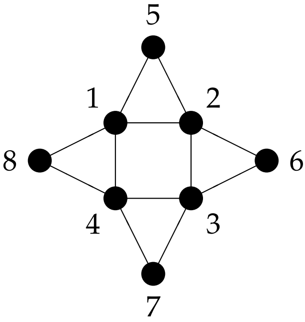

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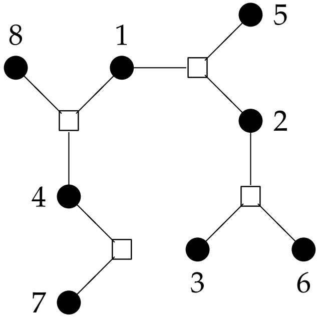

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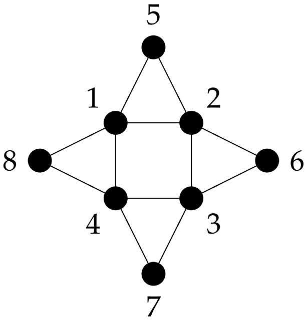

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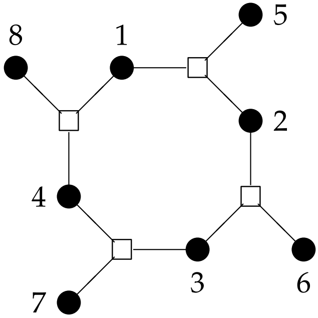

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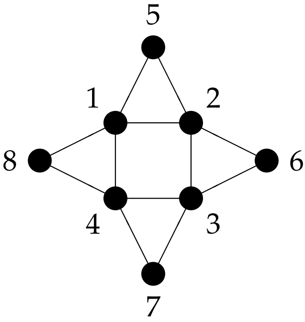

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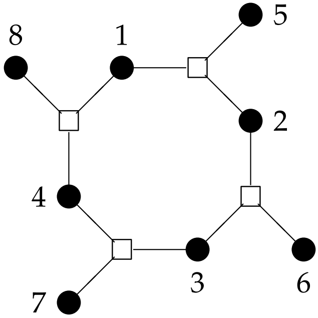

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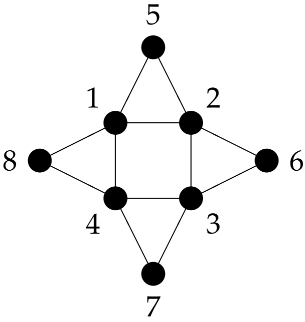

concurrence graph
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E-optimality: the edge-cutset lemma

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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

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

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If c is small but m and n are both large, then θ_1 is small.

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which is at most c is no multiple edges are involved.

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If $m' << m$ and $n' << n$ then θ_1 is small.

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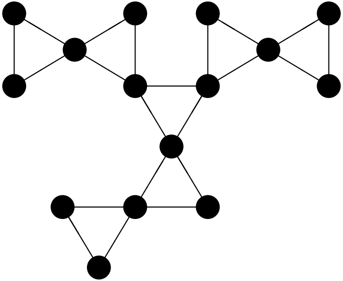

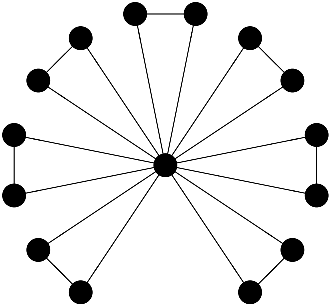

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The concurrence graph is a b-tree of k-cliques,
so the Cutset Lemmas show that
the only E-optimal designs are the queen-bee designs.

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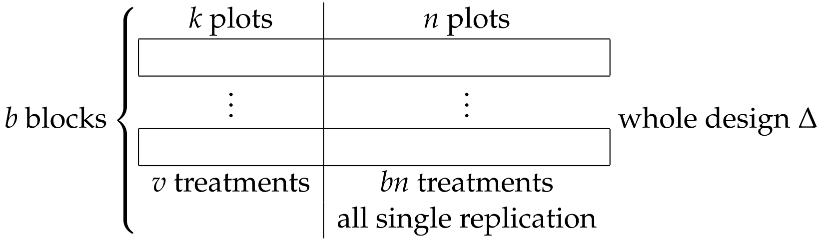
For general block designs, we do not know if we can use the Levi graph to investigate E-optimality.

Large blocks; many unreplicated treatments

Suppose that $\bar{r} = \frac{\sum_i r_i}{v} < 2$.

New conventions: blocks are rows, and block size $= k + n$.



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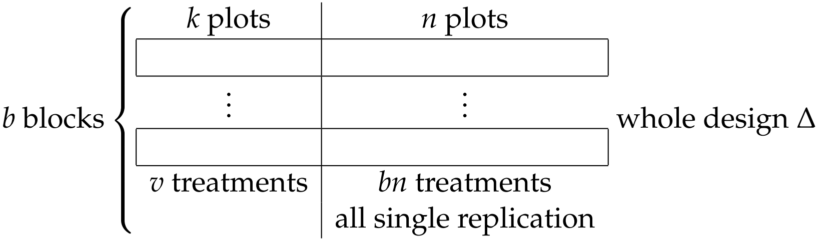

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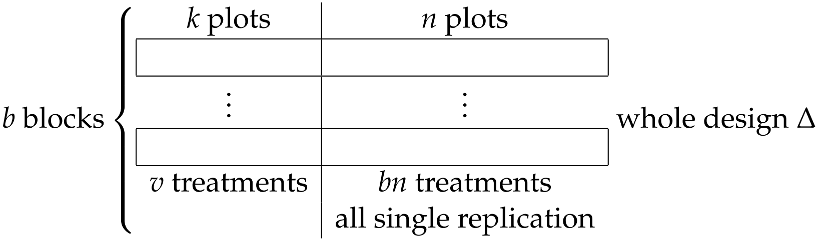

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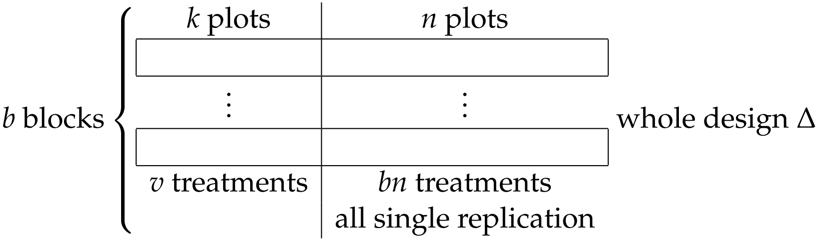
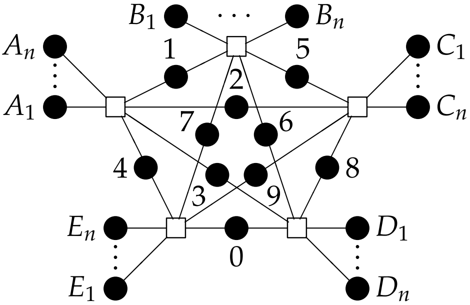


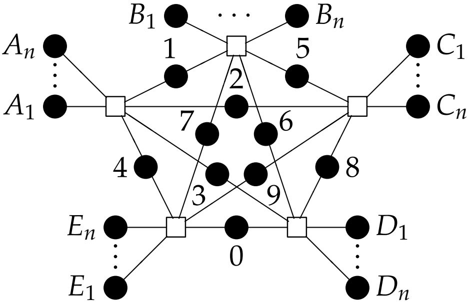
Whole design Δ has $v + bn$ treatments in b blocks of size $k + n$;
the subdesign Γ has v core treatments in b blocks of size k;
call the remaining treatments orphans.

Levi graph: $10 + 5n$ treatments in 5 blocks of $4 + n$ plots

1	2	3	4	A_1	$\cdots$	A_n
1	5	6	7	B_1	$\cdots$	B_n
2	5	8	9	C_1	$\cdots$	C_n
3	6	8	0	D_1	$\cdots$	D_n
4	7	9	0	E_1	$\cdots$	E_n



Pairwise resistance



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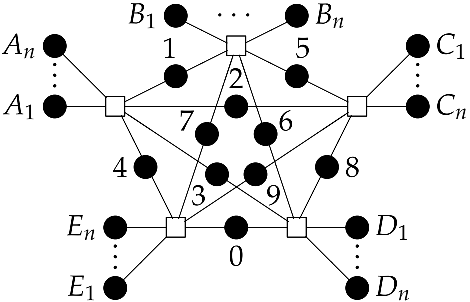

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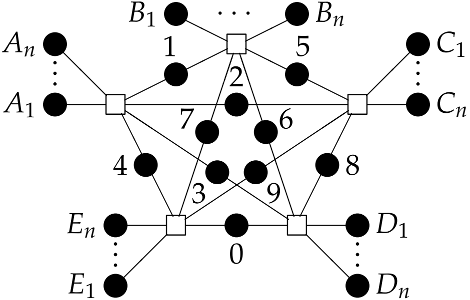

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\text{Resistance}(A_1, A_2) &= 2 \\
\text{Resistance}(A_1, B_1) &= 2 + \text{Resistance}(\text{block } A, \text{block } B) \text{ in } \Gamma
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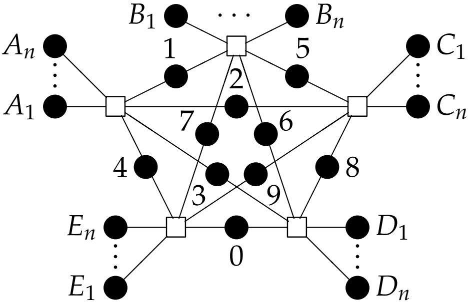

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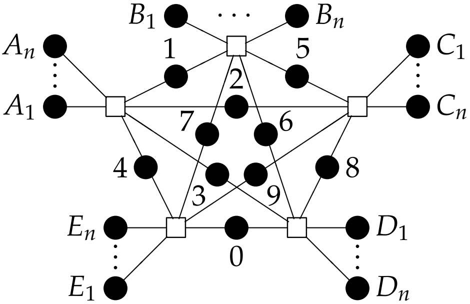

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Sum of the pairwise variances

Theorem (cf Herzberg and Jarrett, 2007)

The sum of the variances of treatment differences in Δ

$$= \textit{constant} + V_1 + nV_3 + n^2V_2,$$

where

$$\begin{aligned} V_1 &= \text{the sum of the variances of treatment differences in } \Gamma \\ V_2 &= \text{the sum of the variances of block differences in } \Gamma \\ V_3 &= \text{the sum of the variances of sums of} \\ &\quad\ \text{one treatment and one block in } \Gamma. \end{aligned}$$

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Consequence

For a given choice of k, make Γ as efficient as possible.

A less obvious consequence

Consequence

If n or b is large,
and we want an A-optimal design,
it may be best to make Γ a complete block design for k' controls,
even if there is no interest in
comparisons between new treatments and controls,
or between controls.

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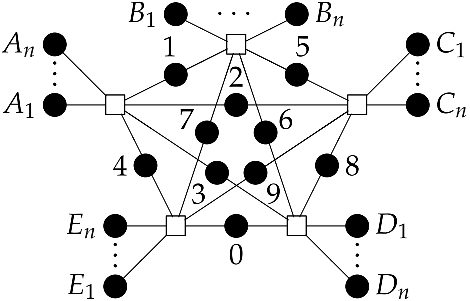

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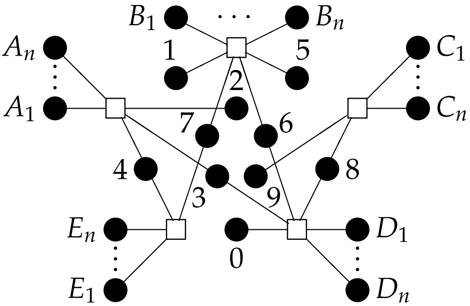

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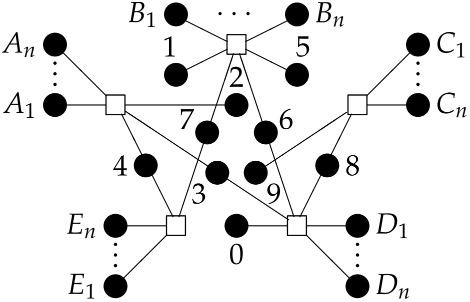

The orphans make no difference to the number of spanning trees for the Levi graph.

D-optimality under very low replication

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The whole design Δ is D-optimal
for $v + bn$ treatments in b blocks of size $k + n$
if and only if the core design Γ is D-optimal
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Consequence

Even when n or b is large,
D-optimal designs do not include uninteresting controls.

Conjectures

Conjecture (Underpinned by theoretical work by C.-S. Cheng)

If the A-optimal design is very different from the D-optimal design, then the E-optimal design is (almost) the same as the A-optimal design.

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Conjecture (Underpinned by theoretical work by J. R. Johnson and M. Walters)

If $\bar{r} > 3.5$ *then designs optimal under one criterion are (almost) optimal under the other criteria.*