Levi graphs and concurrence graphs as tools to evaluate designs

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What makes a block design good for experiments?

I have v treatments that I want to compare.
I have b blocks.
Each block has space for k treatments (not necessarily distinct).

How should I choose a block design?

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

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

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

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n_{ij} = |\{\omega : f(\omega) = i \text{ and } g(\omega) = j\}|
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$=$ number of experimental units in block j which have treatment i.

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

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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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3	3	2
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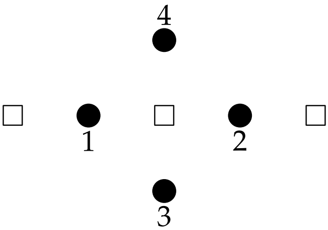

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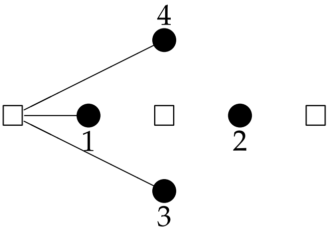

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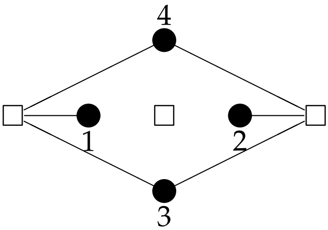

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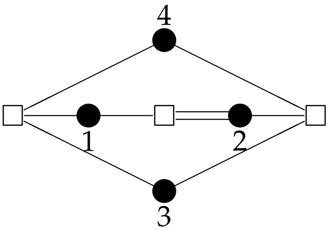

Example 2: $v = 8$, $b = 4$, $k = 3$

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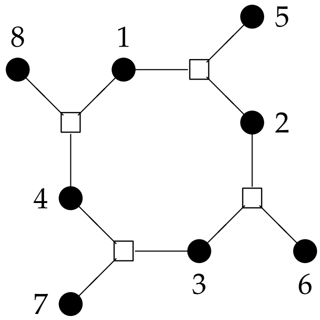

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$$\lambda_{ij} = \sum_{s=1}^{b} n_{is} n_{js};$$

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

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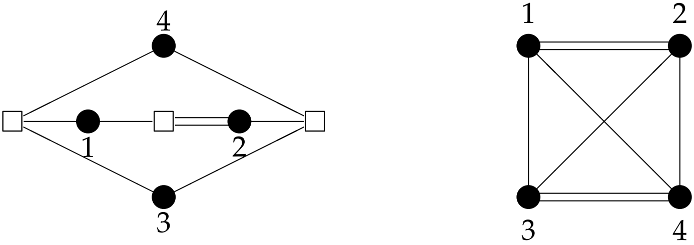

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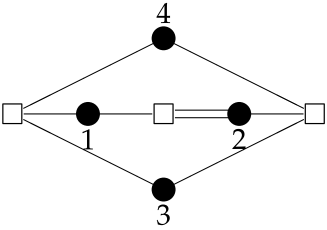
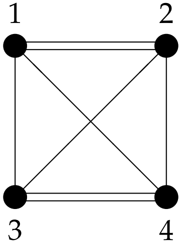


Levi graph
can recover design



concurrence graph
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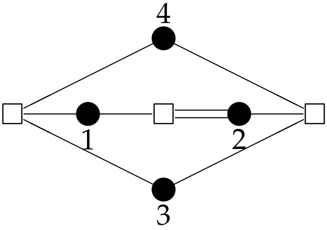

Levi graph
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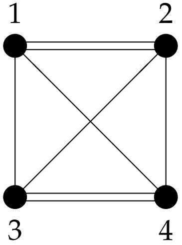

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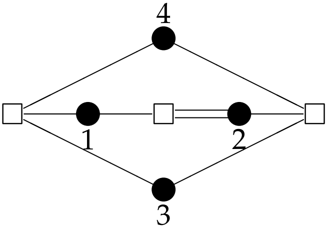

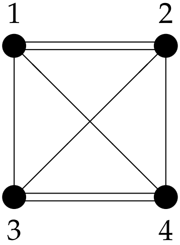

Levi graph
can recover design
more vertices
more edges if $k = 2$

concurrence graph
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more edges if $k \geq 4$

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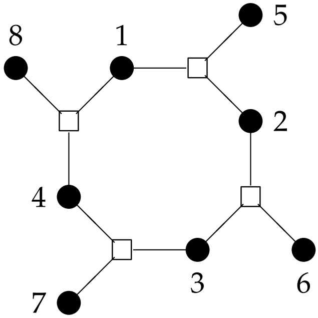

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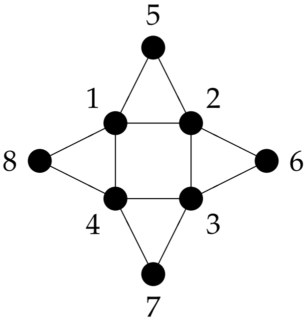

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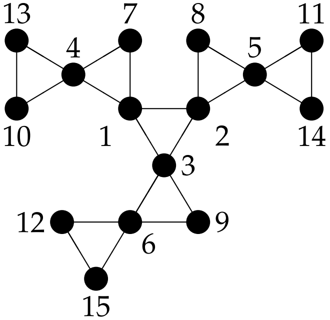

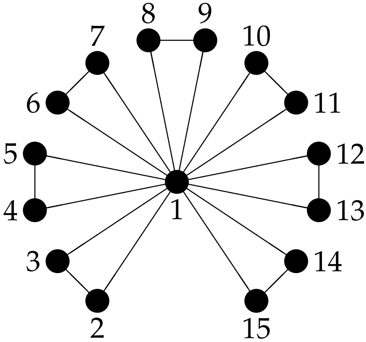

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- $\tilde{L}_{ii} =$ valency of i

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

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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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All row-sums of L and of $\tilde{L}$ are zero,
so both matrices have 0 as eigenvalue
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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.

Generalized inverse

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

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

where J_v is the $v \times v$ all-1 matrix.

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

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We want to estimate contrasts $\sum_i x_i \tau_i$ with $\sum_i x_i = 0$.

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

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

We want all the V_{ij} to be 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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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 $1/I$.

Theorem

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

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

Electrical networks: variance

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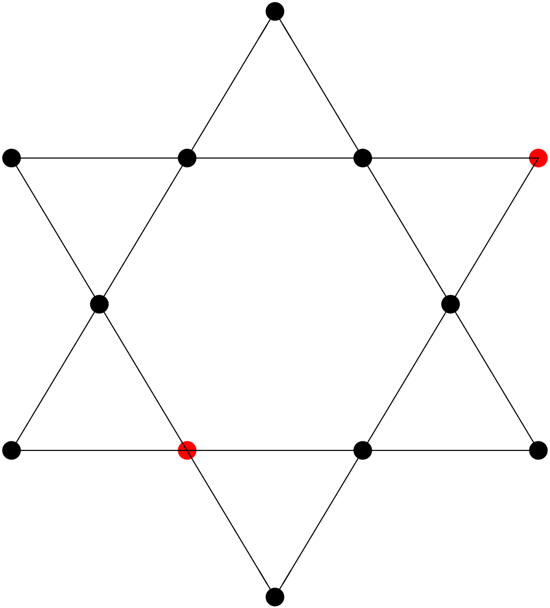
Effective resistances are easy to calculate without matrix inversion if the graph is sparse.

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



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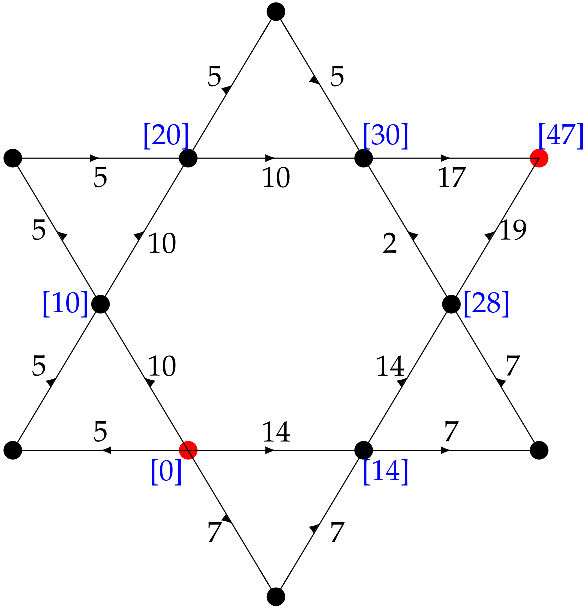

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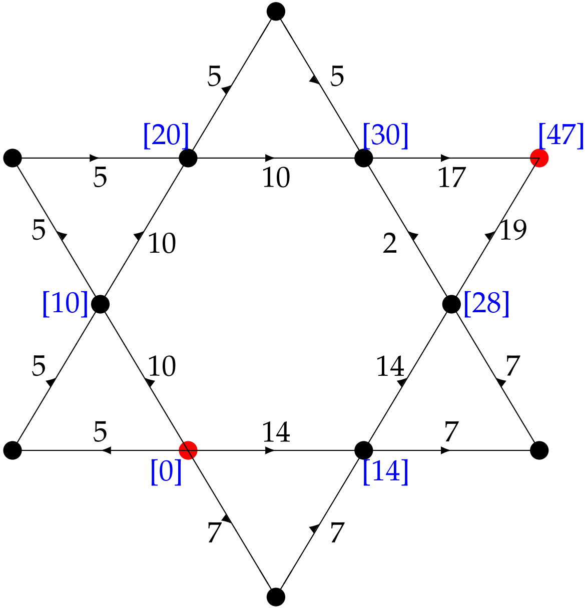

$V = 47$

$I = 36$

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

. . . 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 effective resistance between them in $\tilde{G}$ then

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

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

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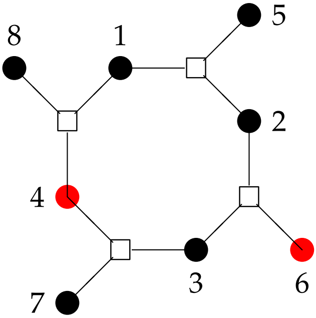

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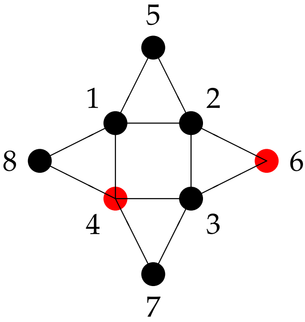

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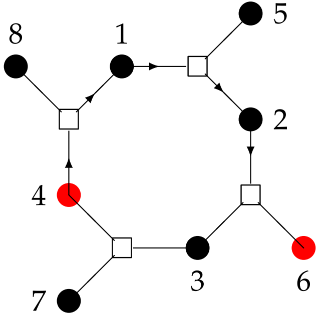
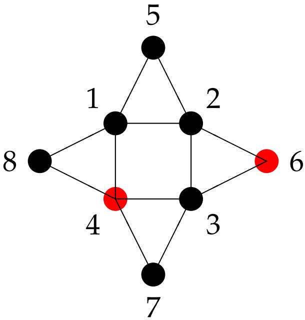


Levi graph



concurrence graph

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

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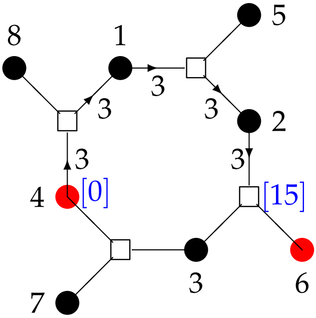

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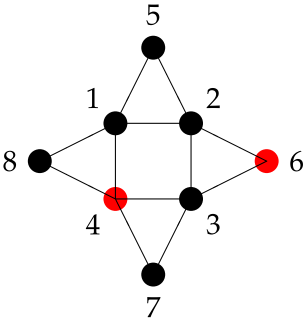

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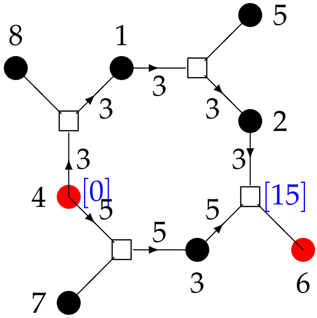

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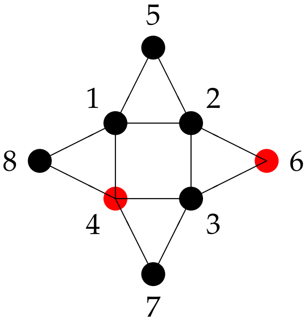

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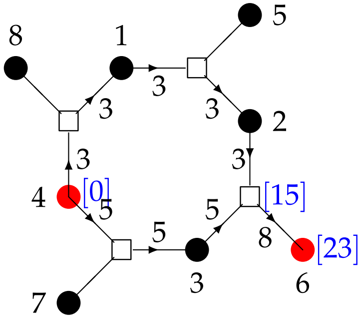

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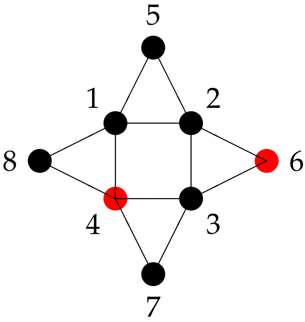

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$$V = 23 \quad I = 8 \quad R = \frac{23}{8}$$

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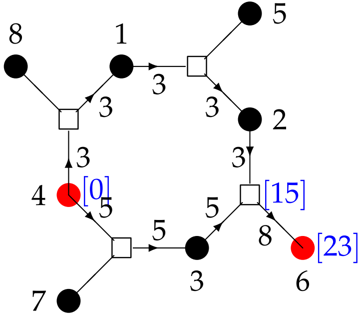

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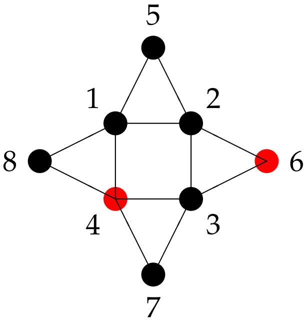

concurrence graph

Resistance increases with distance?

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It is not even true that the largest resistance corresponds to the largest distance in the graph.

Distance-regular graphs

Suppose that the concurrence graph G is simple (no multiple edges).
Let A_d be the $v \times v$ matrix whose (i,j)-entry is equal to

$$\begin{cases} 1 & \text{if the distance from } i \text{ to } j \text{ in } G \text{ is } d \\ 0 & \text{otherwise} \end{cases}$$

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The graph G is distance-regular if $A_1 A_d$ is a linear combination of A_{d-1}, A_d and A_{d+1} for all d.

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Theorem (Biggs)

If G is distance-regular then pairwise resistance is an increasing function of distance.

Anything else nice?

Theorem

If the concurrence graph G is regular
(in particular, if the block design is binary and all treatments have the same replication),
and the Laplacian matrix L has precisely two non-trivial eigenvalues,
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Theorem

If the block design is partially balanced with respect to an amorphic association scheme, then pairwise resistance R_{ij} is a monotonic decreasing function of concurrence λ_{ij}.

Average pairwise variance

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

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

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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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The design is called

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D-optimality: spanning trees

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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
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If $v > b$ it is easier to count spanning trees in the Levi graph than in the concurrence graph.

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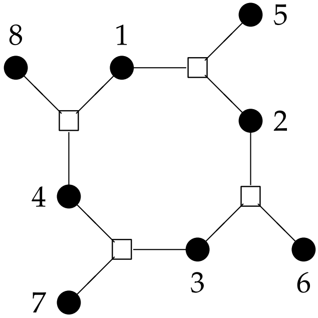

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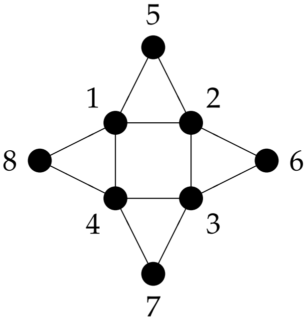

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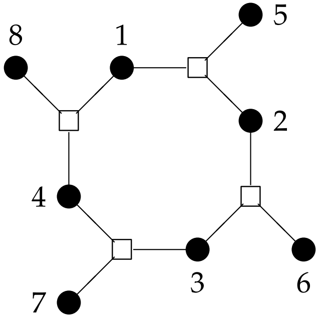

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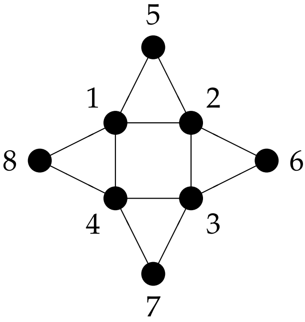

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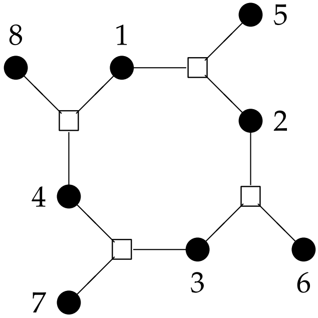

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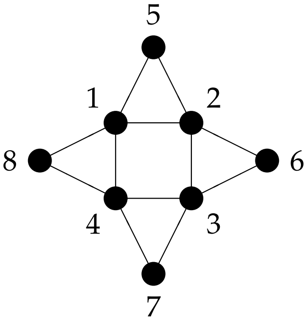

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E-optimality: the cutset lemma

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Lemma

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whose removal separates the graph into components of sizes m and n.
Then

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There is a similar result for vertex-cutsets.

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

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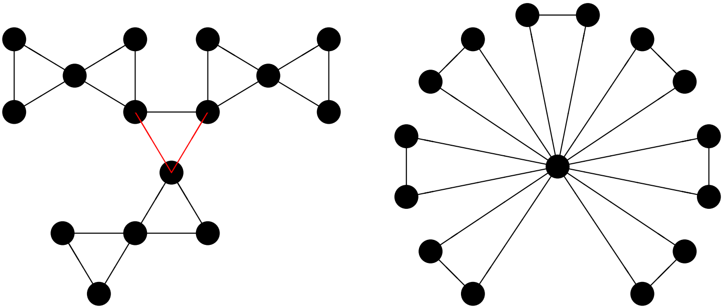

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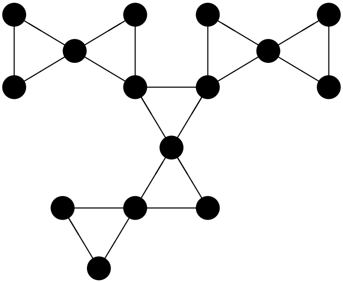

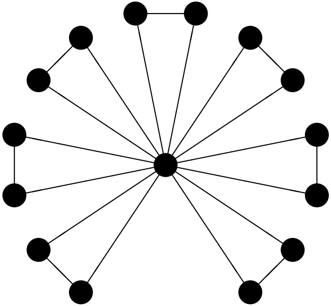

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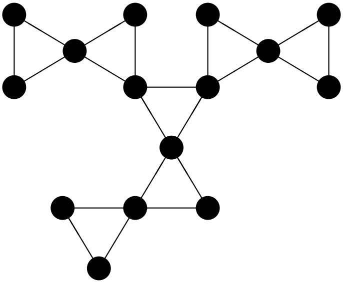

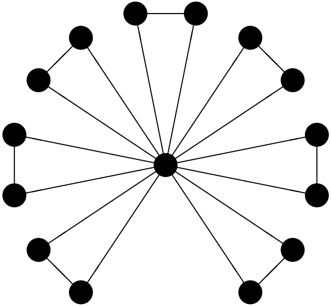

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The only E-optimal designs are the queen-bee designs.

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

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