Conflicts between optimality criteria for block designs with low replication

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Ongoing joint work with Alia Sajjad and Peter Cameron

What makes a block design good for experiments?

I have v treatments that I want to compare.
I have b blocks,
with space for k treatments (not necessarily distinct) in each block.
How should I choose a block design?

Two designs with $v = 5$, $b = 7$, $k = 3$: which is better?

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 is 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.

Design $\longrightarrow$ graph

If $i \neq j$, the concurrence λ_{ij} of treatments i and j is the number of occurrences of the pair $\{i, j\}$ in blocks, counted according to multiplicity.

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The concurrence graph G of the design has the treatments as vertices.
There are no loops.
If $i \neq j$ then there are λ_{ij} edges between i and j.
So the valency d_i of vertex i is

$$d_i = \sum_{j \neq i} \lambda_{ij}.$$

Concurrence graphs of two designs: $v = 15$, $b = 7$, $k = 3$

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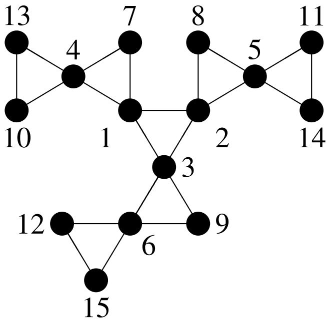

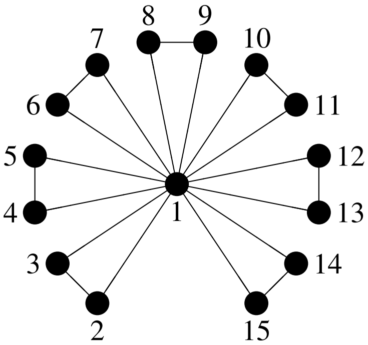

Graph $\longrightarrow$ matrix

The Laplacian matrix L of this graph has

(i,i)-entry equal to $d_i = \sum_{j \neq i} \lambda_{ij}$

(i,j)-entry equal to $-\lambda_{ij}$ if $i \neq j$.

So the row sums of L are all zero.

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$\Longleftrightarrow$ the graph G is connected

$\Longleftrightarrow$ all contrasts between treatment parameters are estimable.

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

Estimation and variance

We measure the response Y on each unit in each block.

If that unit has treatment i and block m, then we assume that

$$Y = \tau_i + \beta_m + \text{random noise.}$$

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*

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

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

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

Optimality

The design is called

- A-optimal if it minimizes the average of the variances V_{ij};

over all block designs with block size k and the given v and b.

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- E-optimal if minimizes the largest value of $x^\top L^- x / x^\top x$;
  —equivalently, it maximizes the minimum non-trivial eigenvalue θ_1 of the Laplacian matrix L:

over all block designs with block size k and the given v and b.

Balanced designs are optimal

Theorem

If there is a balanced incomplete-block design (BIBD) for v treatments in b blocks of size k, then it is A, D and E-optimal.

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Hence a general idea that

- designs optimal on any of these criteria should be close to balanced
- designs optimal on one of these criteria are not very bad on either of the others.

D-optimality: spanning trees

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product of non-trivial eigenvalues of $L = v \times$ number of spanning trees

So a design is D-optimal iff its concurrence graph has the maximal number of spanning trees.

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So a design is D-optimal iff its concurrence graph has the maximal number of spanning trees.

This is easy to calculate by hand when the graph is sparse.

Electrical networks

We can consider the concurrence graph 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: A-optimality

Theorem

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

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

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So

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

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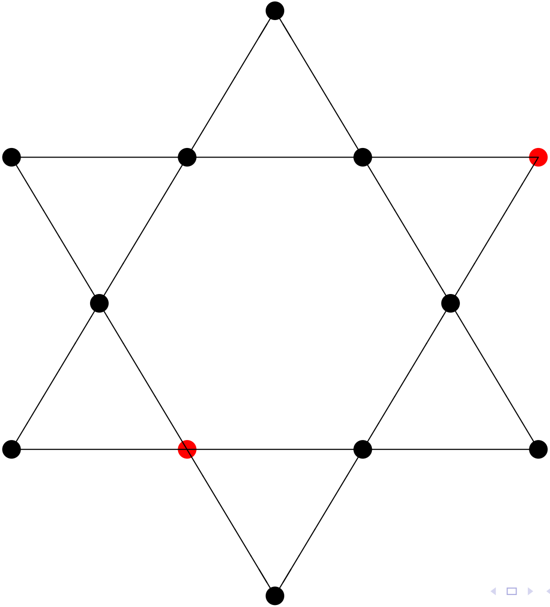
Effective resistances are easy to calculate without matrix inversion if the graph is sparse.

Example calculation



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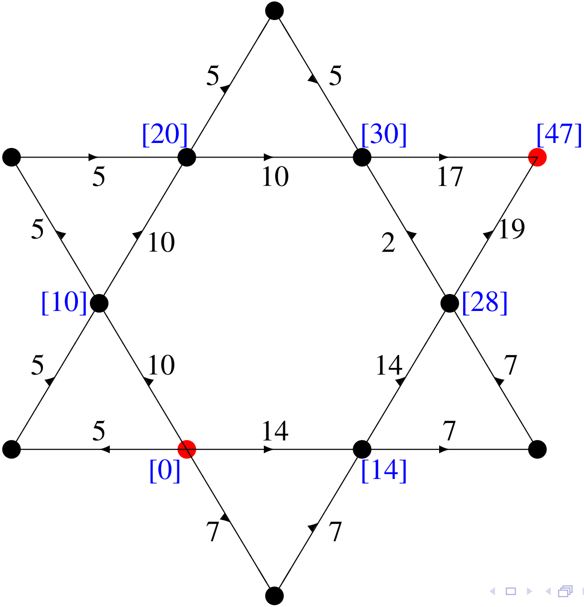

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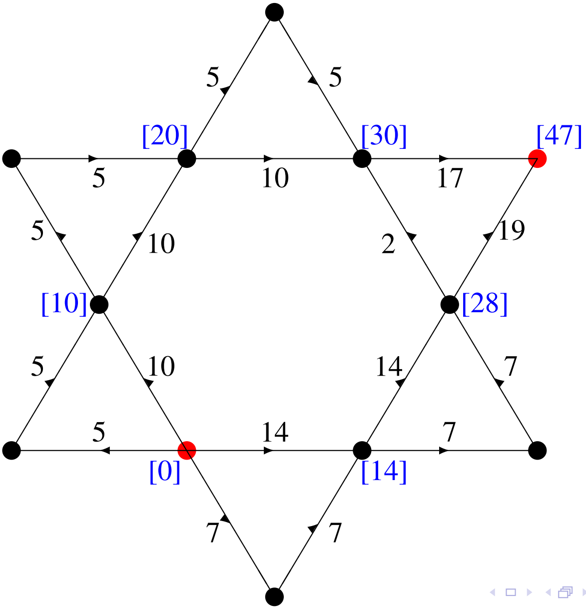

$V = 47$

$I = 36$

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

E-optimality: the cutset lemma

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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Then

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

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

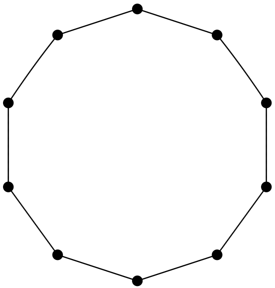
Block size 2: least replication

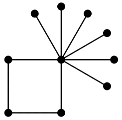
If $k = 2$ then the design is the same as its concurrence graph, and connectivity requires $b \geq v - 1$.

If $b = v - 1$ then all connected designs are trees.
The D-criterion does not differentiate them.
The only A- or E-optimal designs are the stars.

Block size 2: one more block: D

If $k = 2$ and $b = v$ then the design consists of a cycle with trees attached to some vertices.





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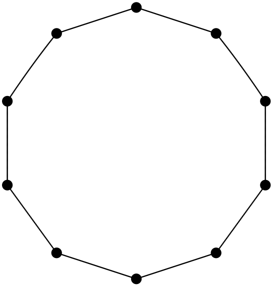
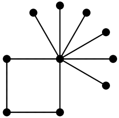
For a spanning tree, remove one edge without disconnecting the graph.





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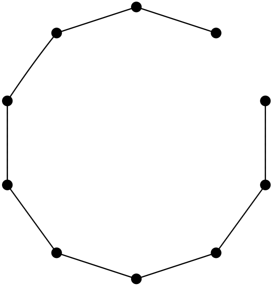

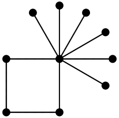

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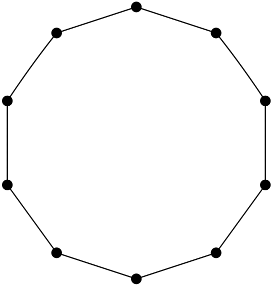

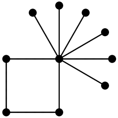

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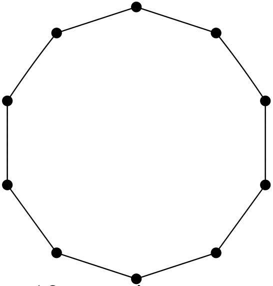
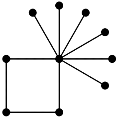


10 spanning trees



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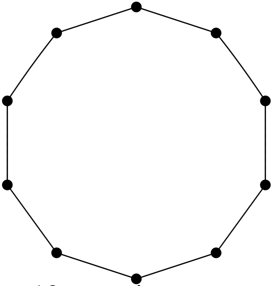

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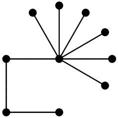

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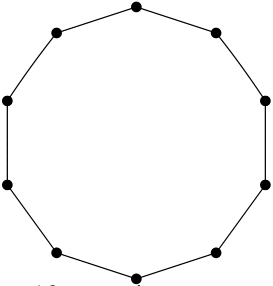

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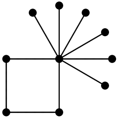

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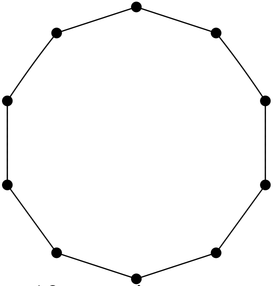

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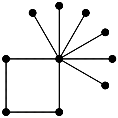
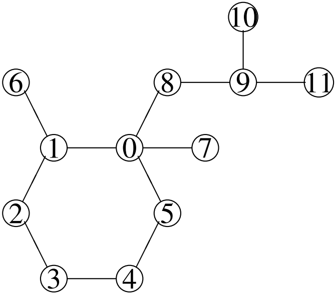
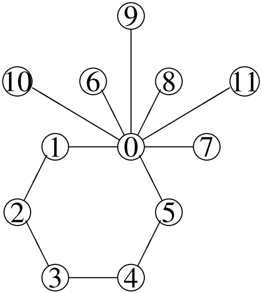


4 spanning trees

The cycle is uniquely D-optimal when $b = v$.

Block size 2: one more block: A and E





For a given size of cycle,
the total variance is minimized
and the smallest non-trivial Laplacian eigenvalue is maximized
when everything outside the cycle is attached as a leaf to the same vertex of the cycle.

Block size 2: one more block

D-optimal designs	cycle	always
A-optimal designs	cycle	if $v \leq 8$
	square with leaves attached	if $9 \leq v \leq 12$
	triangle with leaves attached	if $12 \leq v$
E-optimal designs	cycle	if $v \leq 6$
	triangle or digon with leaves	if $6 \leq v$

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For $v \geq 9$, the ranking on the D-criterion is essentially the opposite of the rankings on the A- and E-criteria.

A statistician says . . .

An old collaborator, 1980s

"We all know that the A-optimal designs are essentially the same as the D-optimal designs.

Surely you've got enough mathematics to prove this?"

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That old collaborator, December 2008

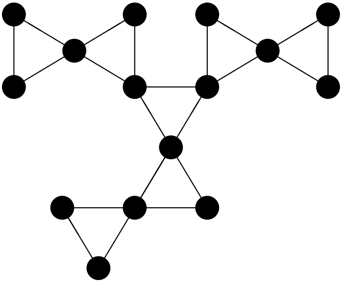
"It seems to be just block size 2 *that is a problem."*

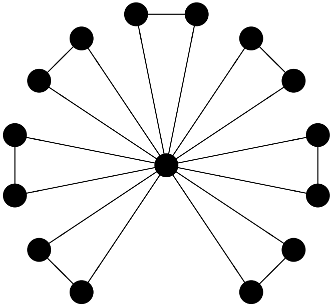
Block size 3, but minimal b

The remaining arguments extend easily to general block size.

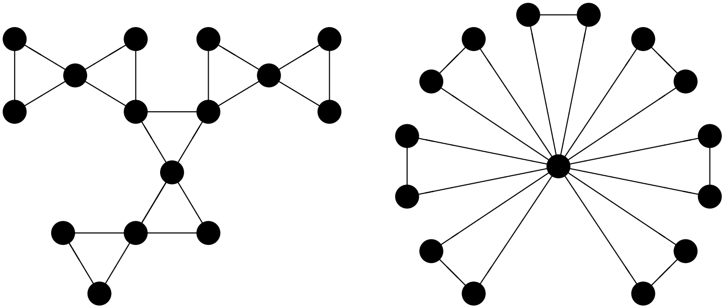
When $k = 3$, for a connected design, we need $2b \geq v - 1$.

If $2b + 1 = v$ then all designs are gum-trees, in the sense that there is a unique sequence of blocks from any one treatment to another.

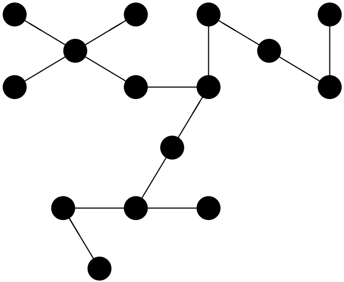


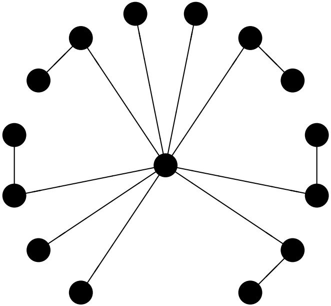


Block size 3, but minimal b: D

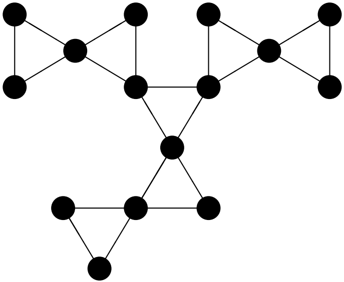


Block size 3, but minimal b: D

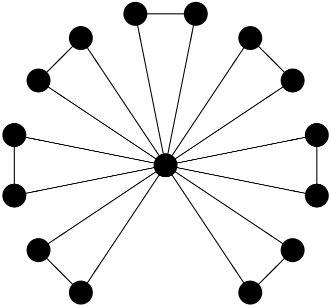




Block size 3, but minimal b: D



3^7 spanning trees



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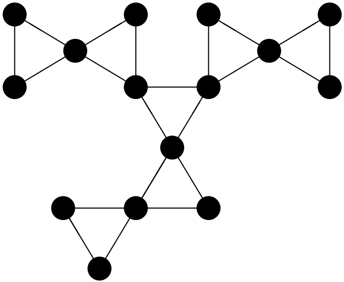

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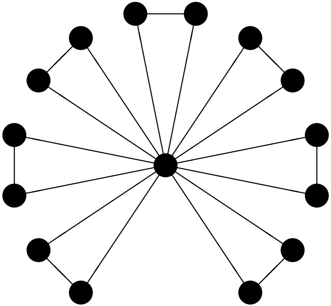
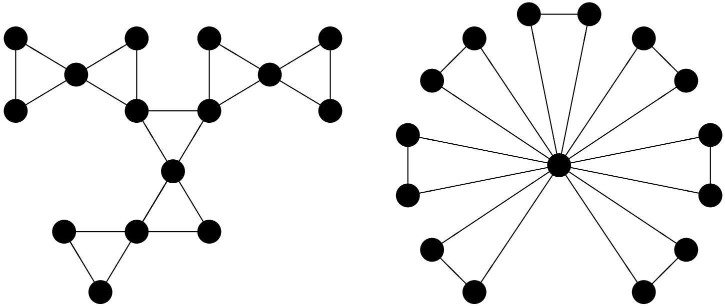


3^7 spanning trees

Every gum-tree with b blocks of size 3 has 3^b spanning trees.
The D-criterion does not differentiate them.

Block size 3, but minimal b: A



Let R_{ij} be the effective resistance between treatments i and j.

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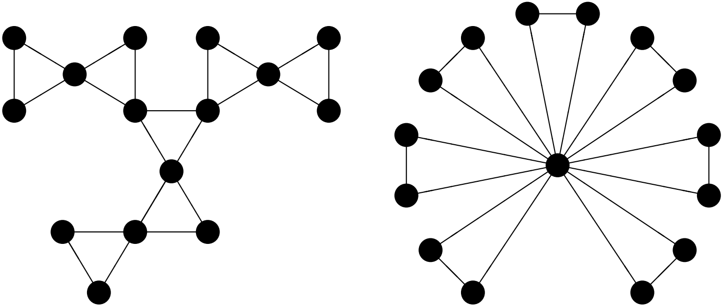

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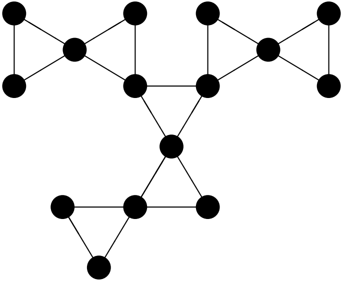

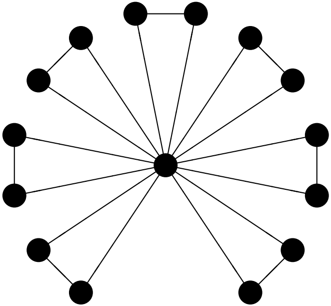

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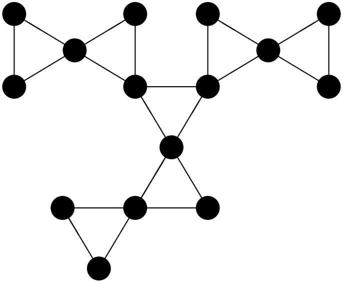 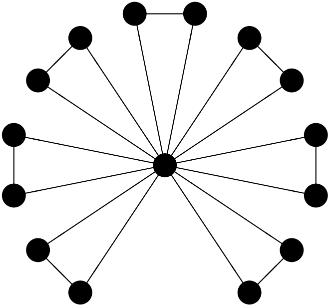

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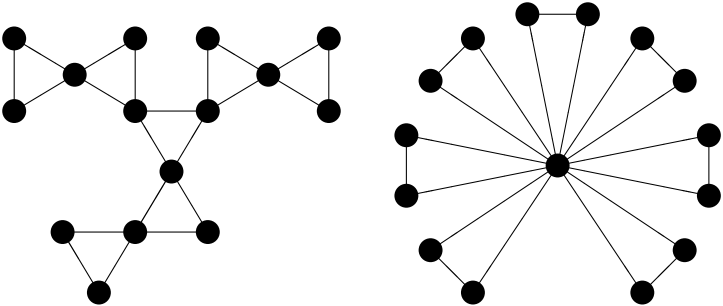

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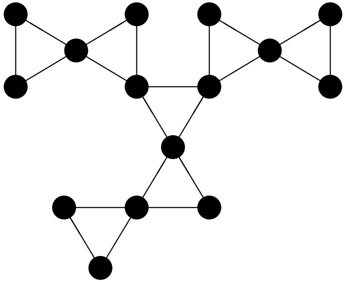
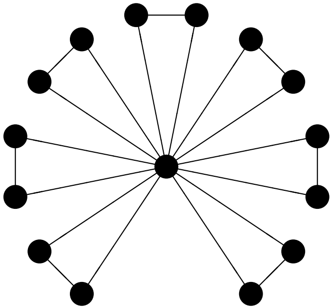
The only A-optimal designs are the queen-bee designs.

Block size 3, but minimal b: E





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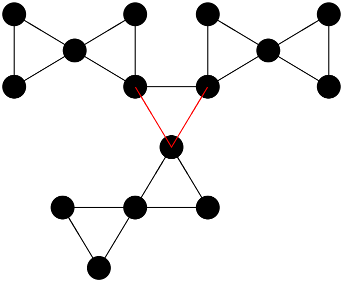
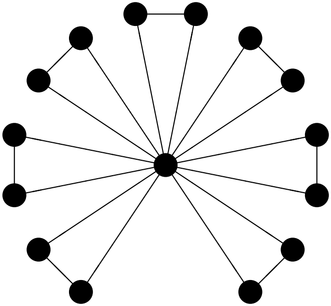


$$\theta_1 \leq 2\left(\frac{1}{5} + \frac{1}{10}\right)$$



$$\theta_1 \geq 1$$

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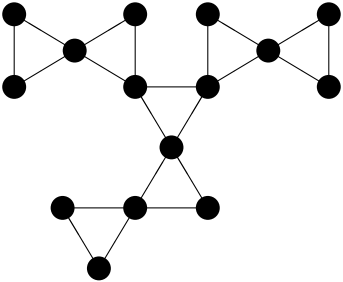
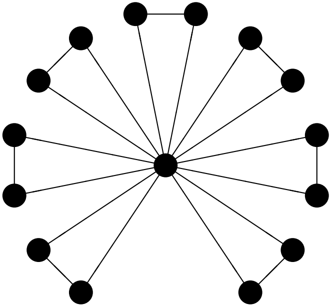


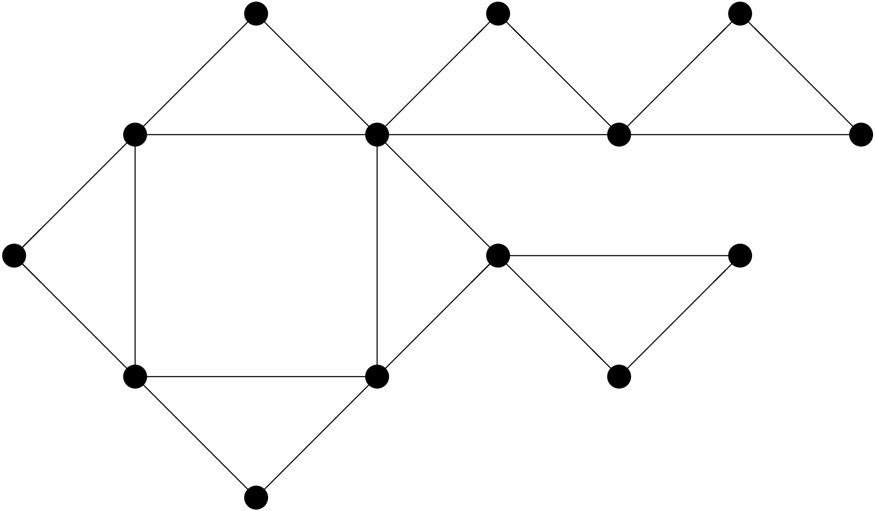


$$\theta_1 \leq 2\left(\frac{1}{5} + \frac{1}{10}\right) \qquad\qquad \theta_1 \geq 1$$

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

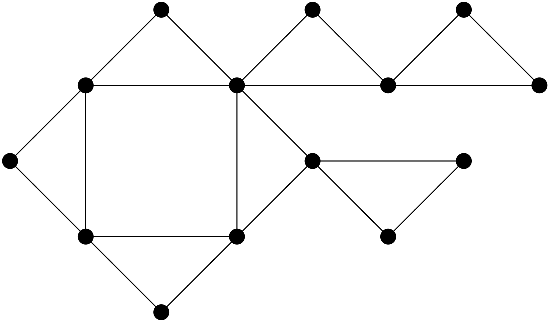
Block size 3, but $b =$ minimal $+1$

If $2b = v$ then G is a gum-cycle with gum-trees attached.



Block size 3, but $b =$ minimal $+1$: D

Suppose that there are s blocks in the gum-cycle.



Block size 3, but $b =$ minimal $+1$: D

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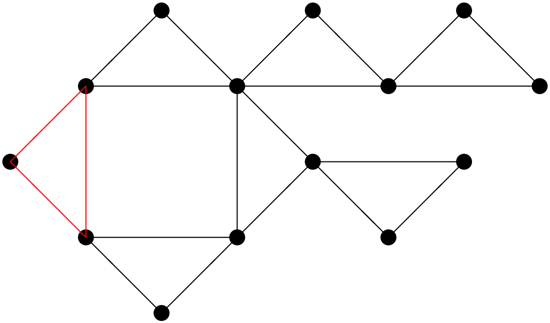

For a spanning tree:
choose a block in the gum-cycle s

Block size 3, but $b =$ minimal $+1$: D

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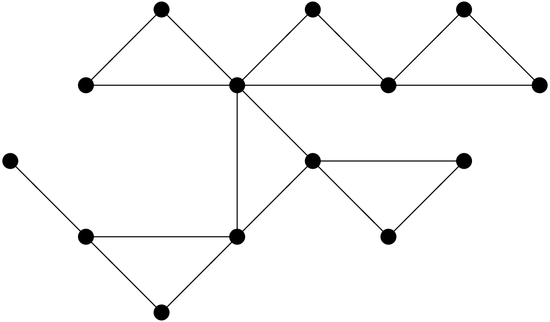

For a spanning tree:

choose a block in the gum-cycle	s
remove its central edge and one other	2

Block size 3, but $b =$ minimal $+1$: D

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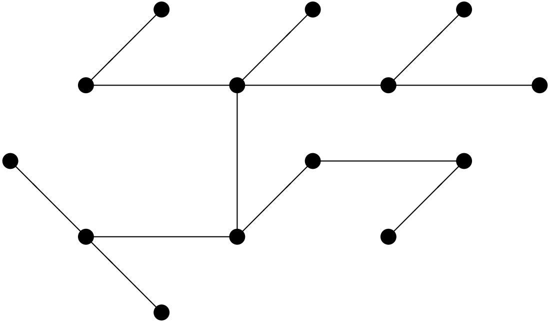

For a spanning tree:

choose a block in the gum-cycle	s
remove its central edge and one other	2
remove an edge from each other block	3^{b-1}

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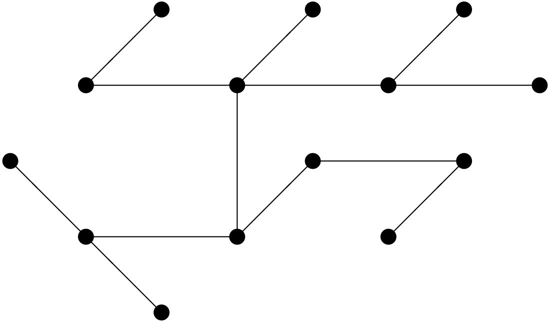

For a spanning tree:

choose a block in the gum-cycle	s
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There are $2s \times 3^{b-1}$ spanning trees.

This is maximized when $s = b$.

Block size k, but $b =$ minimal $+1$: D-optimality

This argument extends to all block sizes.

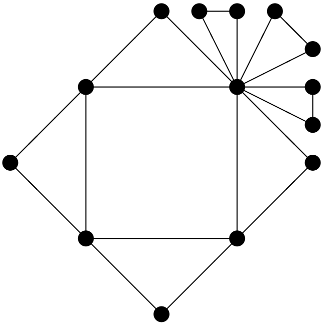
If $v = b(k-1)$ then the only D-optimal designs are the gum-cycles.

Block size 3, but $b =$ minimal $+1$: A

Suppose that there are s blocks in the gum-cycle.

Block size 3, but $b =$ minimal $+1$: A

Suppose that there are s blocks in the gum-cycle.
Then the only candidate for A-optimality consists of $b - s$ triangles attached to a central vertex of the gum-cycle.



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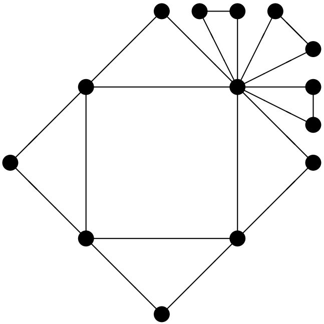

The sum of the pairwise effective resistances is a cubic function of s.

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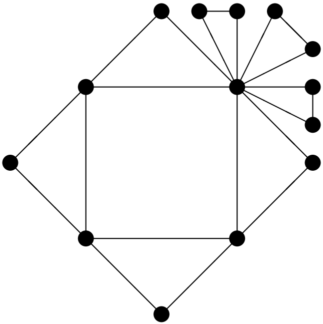

The sum of the pairwise effective resistances is a cubic function of s.

The location of the minimum on $[2, b]$ depends on the value of b.

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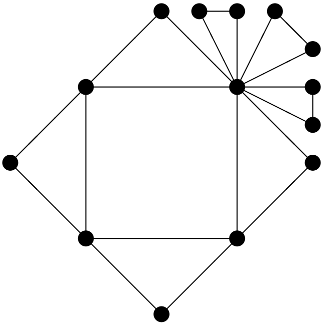

The sum of the pairwise effective resistances is a cubic function of s.

The location of the minimum on $[2,b]$ depends on the value of b.

A-optimal designs do not have s large.

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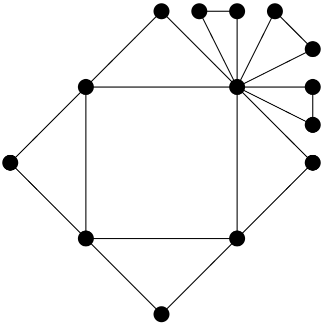

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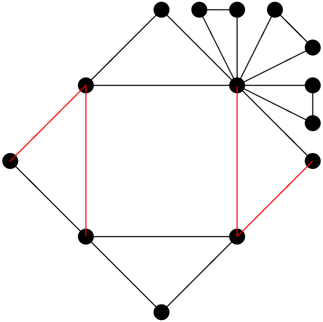

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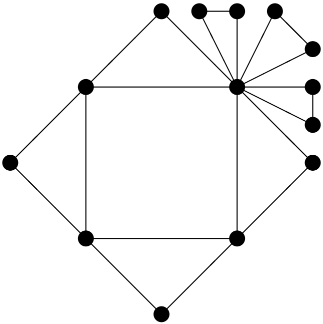

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New asymptotic results (large v)

Current work by J. Robert Johnson and Mark Walters.

Block size 2; one control treatment; want to minimize the average variance of comparisons with control.

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Average replication	optimal design (probably)
2 and a little above	many small designs (including many leaves) glued at the control
around 3	one large random almost-regular graph with average replication 3.5, also quite a lot of edges from points in this to the control, and a bunch of leaves rooted at the control
4 and above	a random almost-regular graph (maybe with a few leaves)