Can algebraic graph theory help to find good block designs for experiments?

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QMUL (emerita)

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Motivation: I

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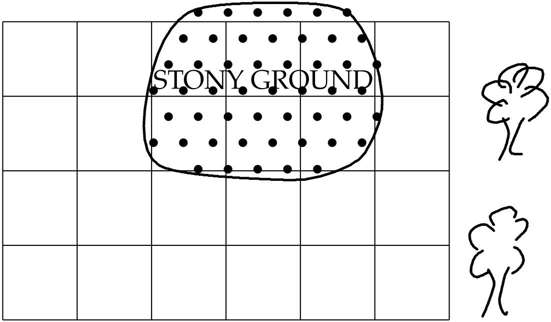
In his talk on 4 November, Misha Muzychuk asked

> *"What insights or problems can algebraic graph theorists gain from work in statistics?"*

Example: an experiment in a field

We have 6 varieties of cabbage to compare in this field.
How do we avoid bias?



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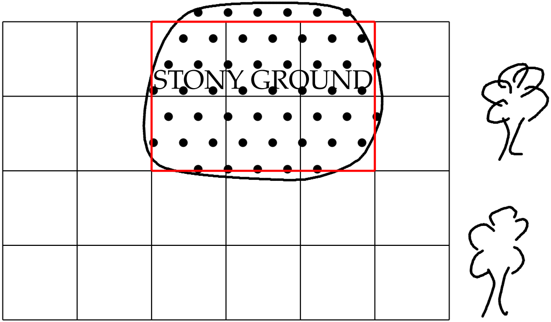

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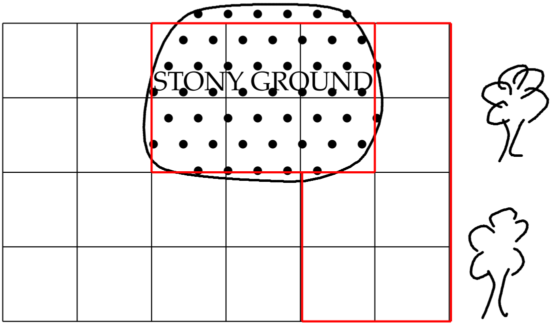

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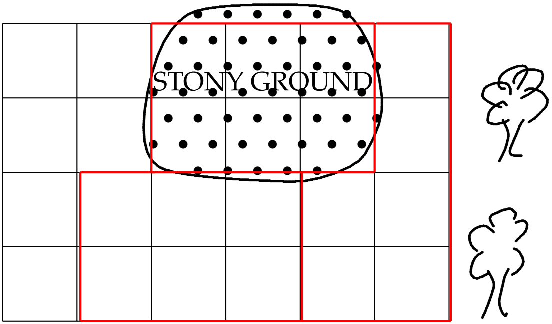

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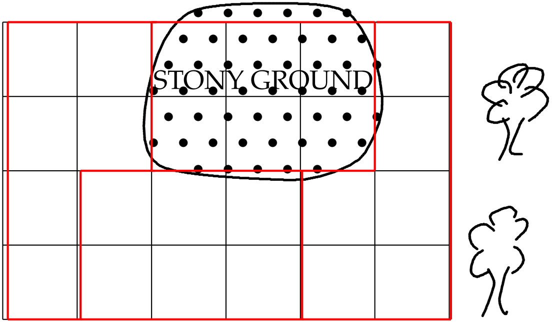

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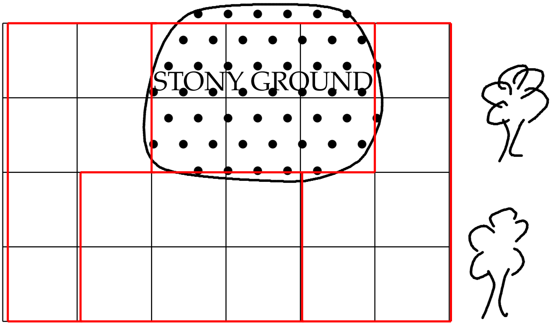

Partition the experimental units into homogeneous blocks and plant each variety on one plot in each block.

Experiments in blocks

I have v treatments that I want to compare.
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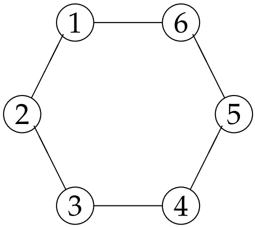
What makes a block design good?

Two designs for 6 treatments in 6 blocks of size 2 (shown with edges as blocks). Which is better?



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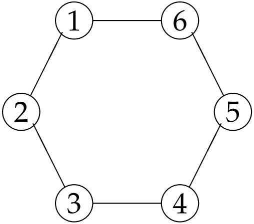

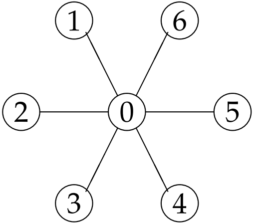

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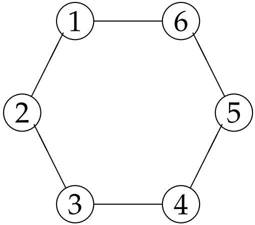

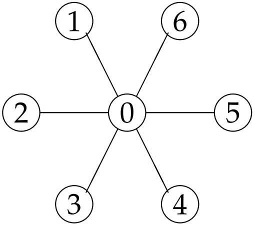

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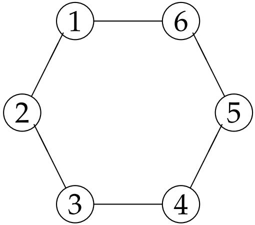

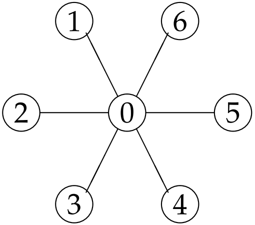

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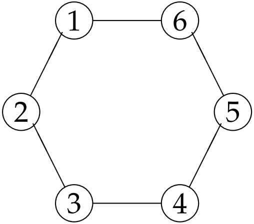

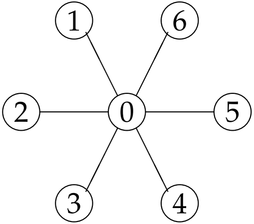

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Biologists know that they should compare all treatments with the same thing.

They should not test treatment 6 now and compare the results with testing treatment 1 ten years ago.

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

Conventions: columns are blocks
(sometimes rows, but the boxes should make it clear);
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
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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.

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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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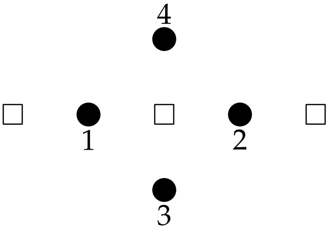

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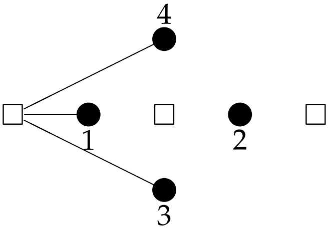

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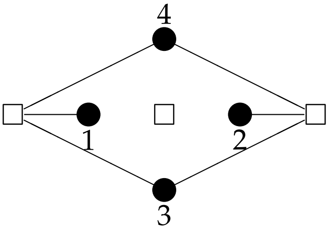

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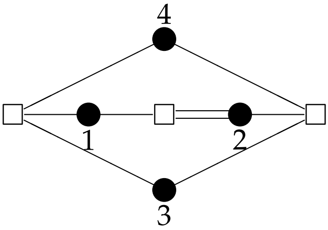

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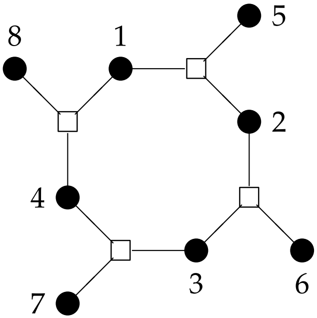

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$$\lambda_{ij} = \sum_{s=1}^{b} n_{is} n_{js};$$

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

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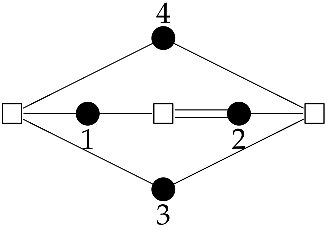

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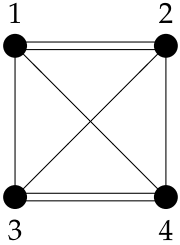

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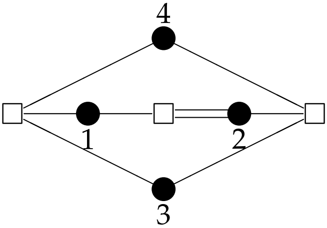
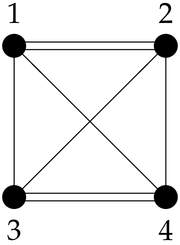


Levi graph
can recover design



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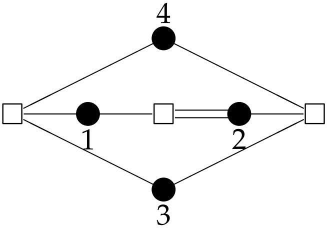

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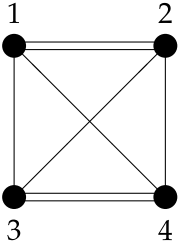

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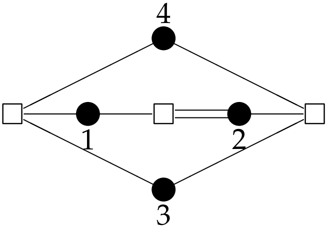

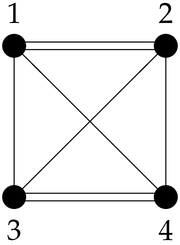

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more vertices
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concurrence graph
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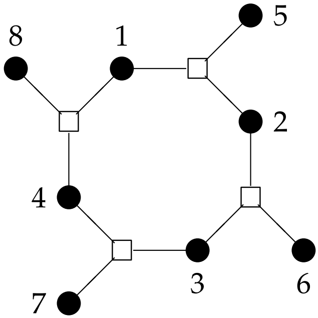

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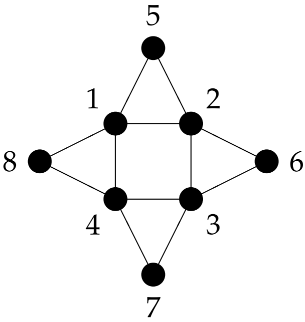

concurrence graph

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

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

1	1	1	1	1	1	1
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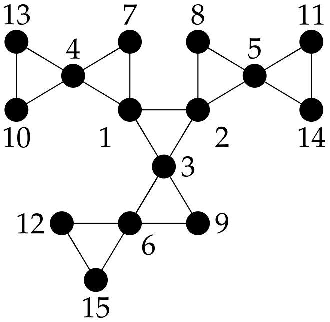

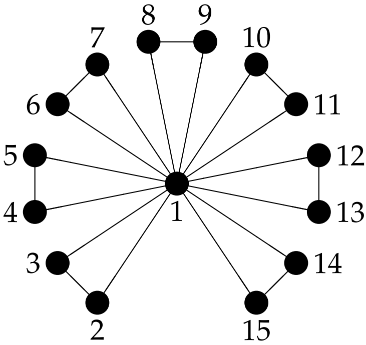

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- $\tilde{L}_{ii} = \text{valency of } i$

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

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

The Laplacian matrix $\tilde{L}$ of the Levi graph $\tilde{G}$ is a $(v+b) \times (v+b)$ matrix with (i,j)-entry as follows:

- $\tilde{L}_{ii} = \text{valency of } i$
  $$= \begin{cases} k & \text{if } i \text{ is a block} \\ \text{replication } r_i \text{ of } i & \text{if } i \text{ is a treatment} \end{cases}$$
- if $i \neq j$ then $L_{ij} = -(\text{number of edges between } i \text{ and } j)$

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

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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.

(The matrix $\frac{1}{v}J_v$ is the orthogonal projector onto the null space of L.)

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

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: effective resistance

Theorem

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

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

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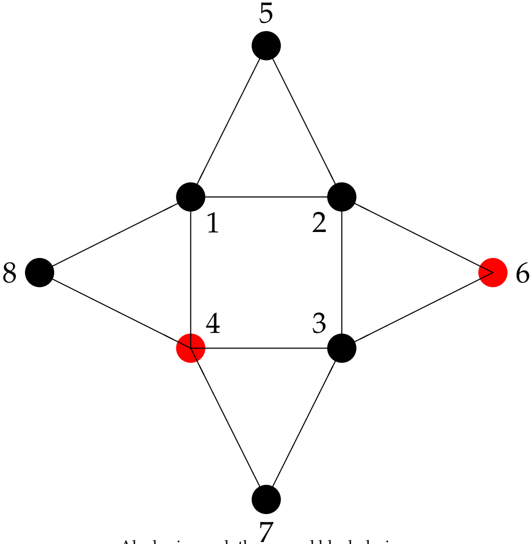
Effective resistances are easy to calculate without matrix inversion if the graph is sparse.

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



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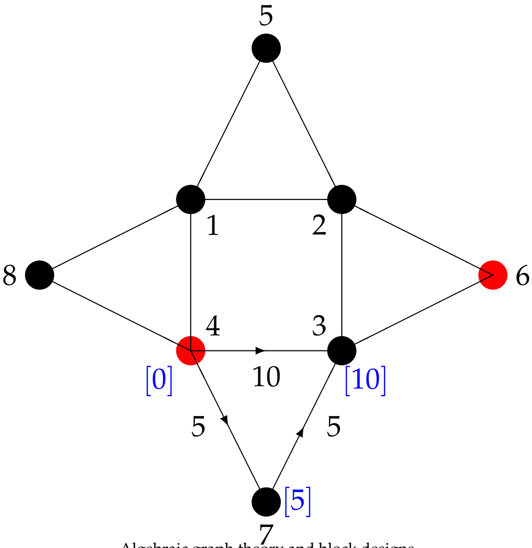

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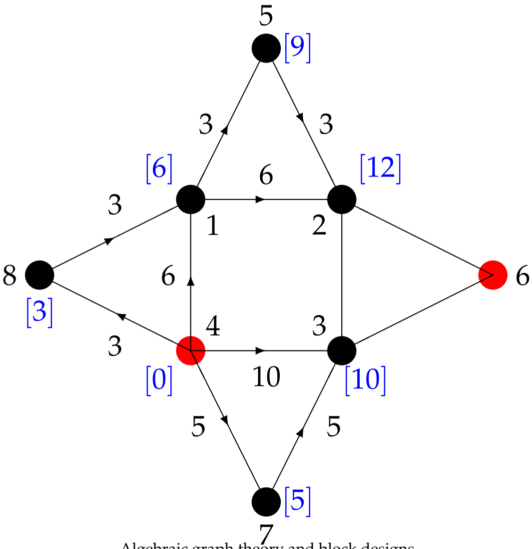

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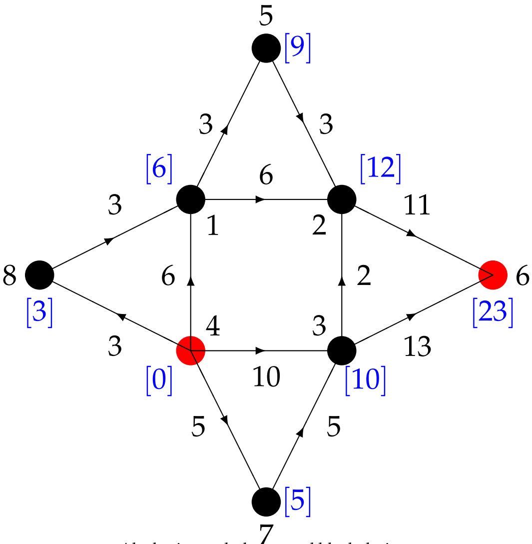

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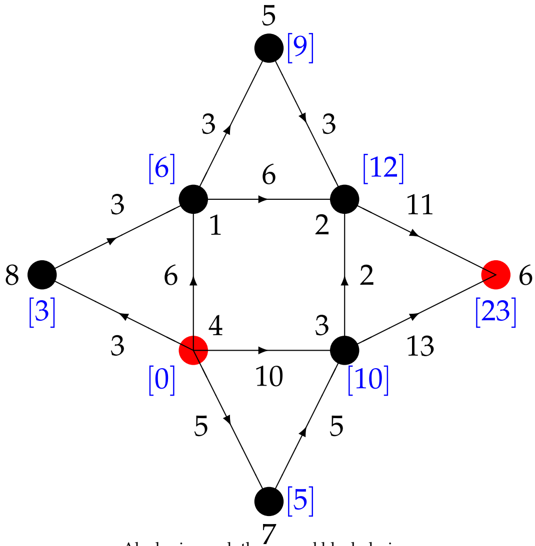
$$V = 23 \quad I = 24 \quad R = \frac{23}{24}$$



. . . Or we can use the Levi graph

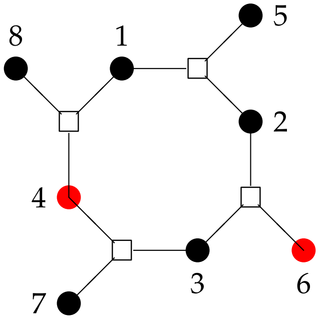
Theorem

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

$$\tilde{R}_{ij} = kR_{ij}.$$

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

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



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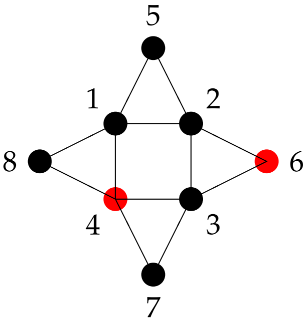

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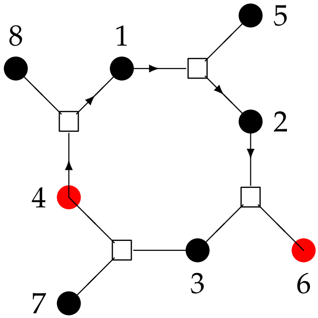

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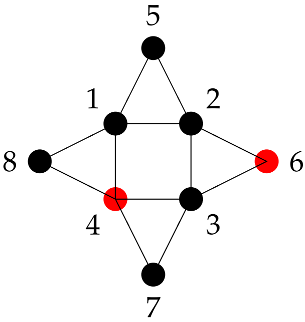

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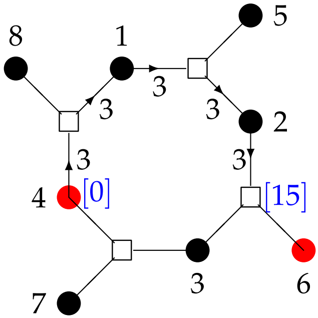

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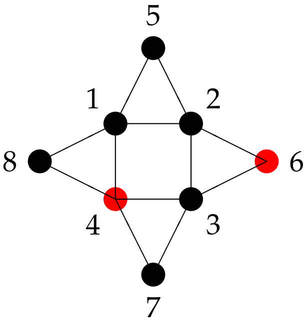

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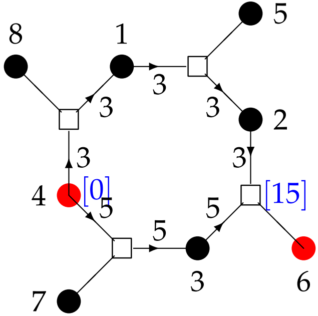

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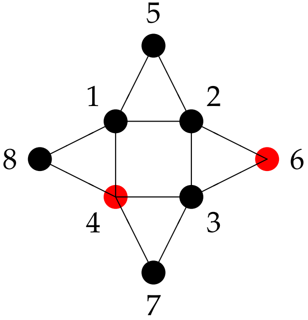

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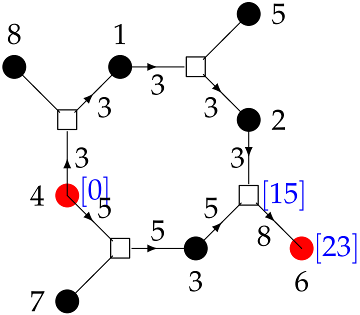

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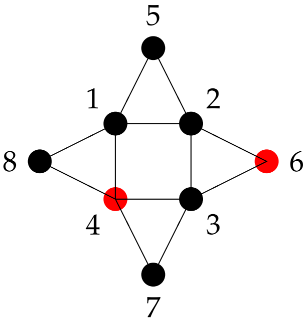

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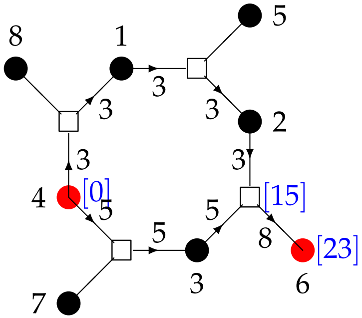

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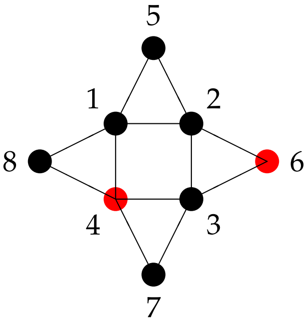

concurrence graph

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

Spanning trees

A spanning tree for a 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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Theorem (Gaffke, 1982)

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

BIBDs are optimal

Theorem (Kshirsagar, 1958; Kiefer, 1975)

If there is a balanced incomplete-block design (BIBD) (2-design) for v treatments in b blocks of size k, then it is A- and D-optimal. Moreover, no non-BIBD is A- or D-optimal.

Folklore

For decades, it was assumed that, for given values of v, b and k,

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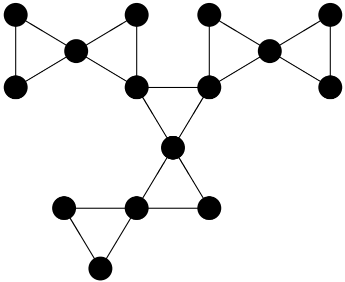

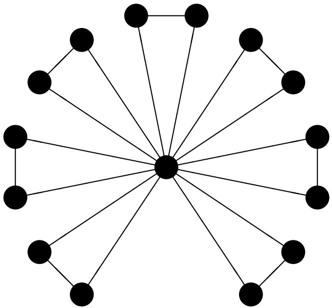

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The Levi graph is a tree,
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The Levi graph is a tree,
so effective resistance = graph distance,
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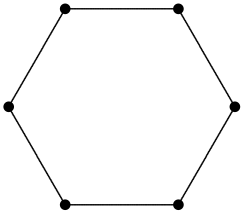
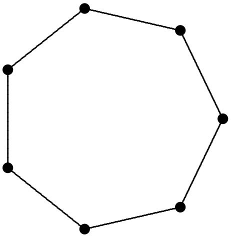
Each spanning tree is made by removing a single edge from the cycle, so the D-optimal designs are those in which the maximum number of edges are in the cycle.

A-optimal designs when $k = 2$ and $b = v$

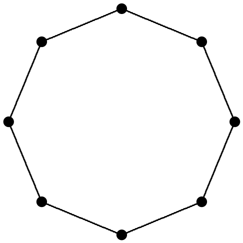
$v = 6$



$v = 7$



$v = 8$



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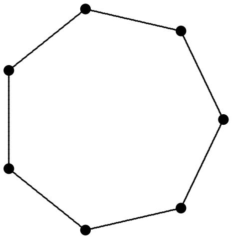
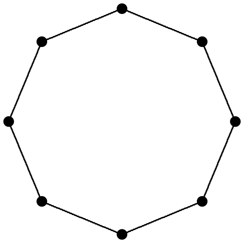
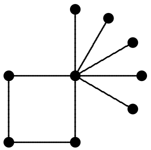
$v = 7$ $v = 8$ $v = 9$







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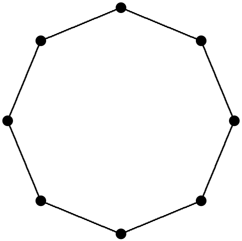
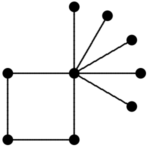
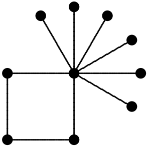


$v = 9$



$v = 10$



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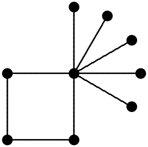

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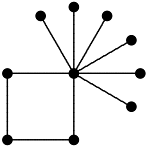
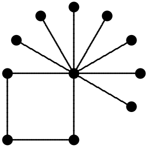


$v = 11$



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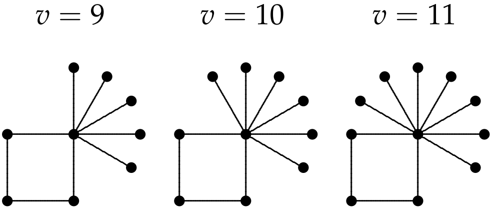

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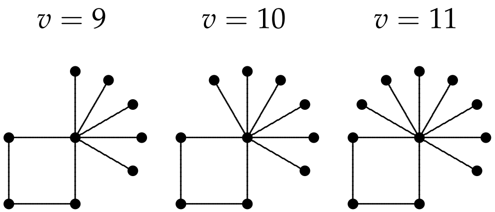
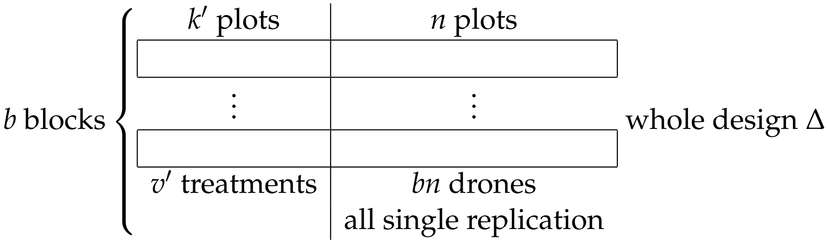


For $v \geq 13$ the A-optimal design is a triangle with all other edges adjacent to a single vertex of the triangle.
For $v = 12$, the cycle can be either a triangle or a square.

Large blocks; many unreplicated treatments

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

Blocks are rows, treatments with single replication are drones.



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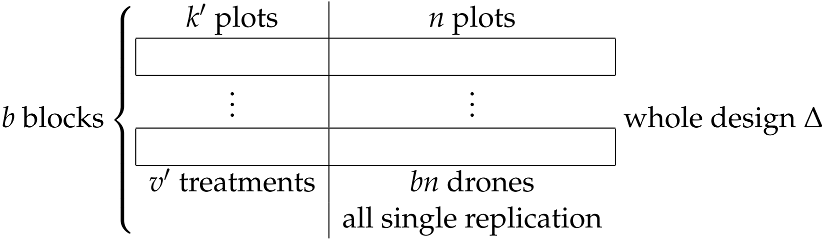

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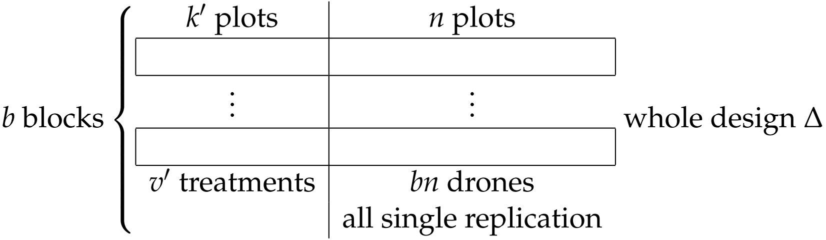

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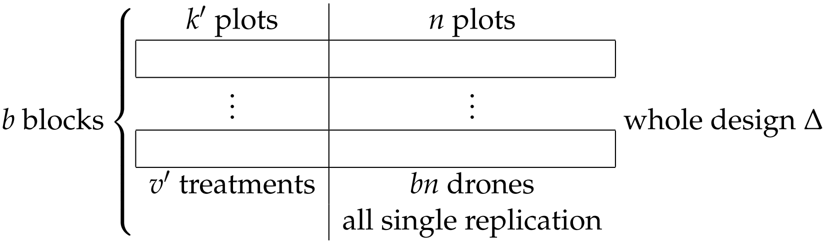

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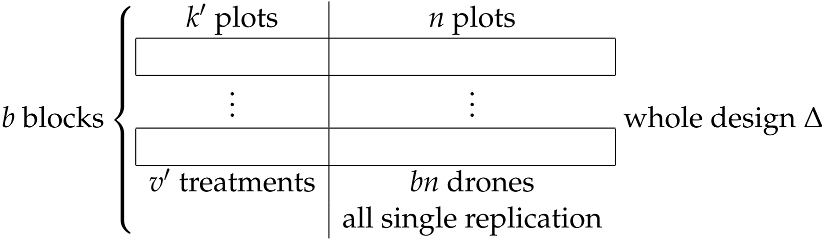

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$$n \geq n_0 = \left\lfloor \frac{2v - bk}{b} \right\rfloor$$

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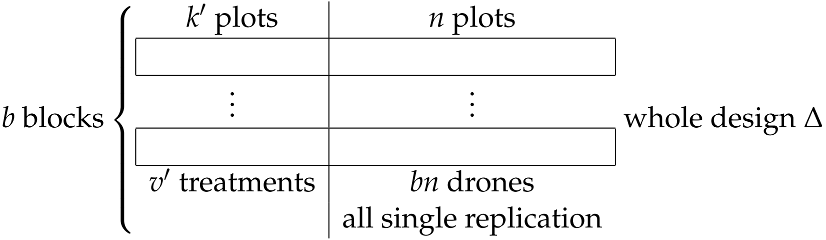
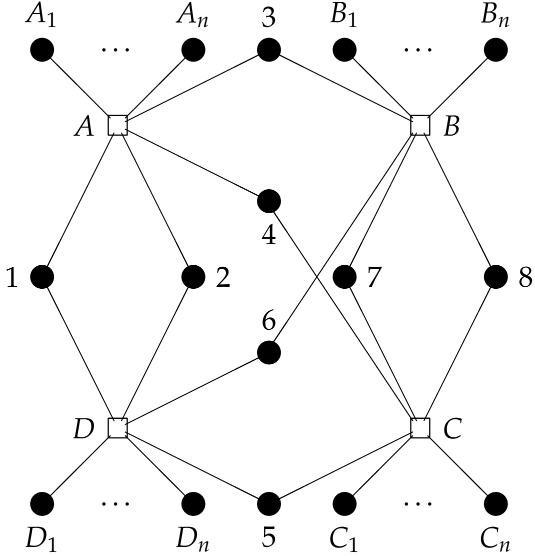
Suppose that $\bar{r} = \frac{\sum_i r_i}{v} < 2$.

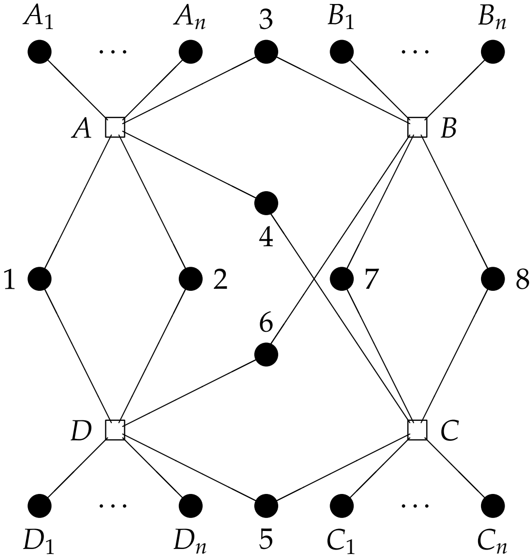
Blocks are rows, treatments with single replication are drones.



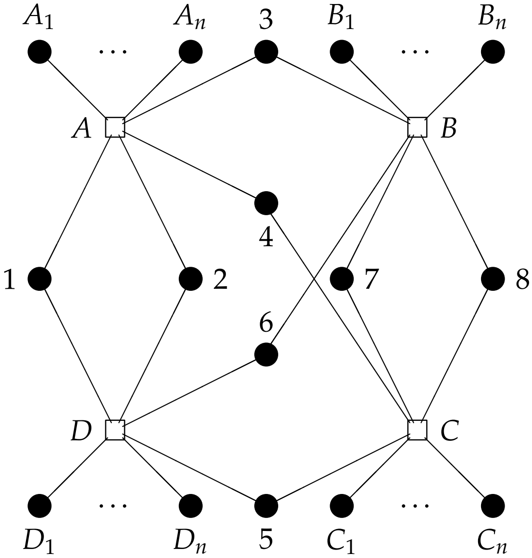
Whole design Δ has v treatments in b blocks of size $k = k' + n$;
the subdesign Γ has v' core treatments in b blocks of size k'.
(The core treatments may include extra drones.)

$$n \geq n_0 = \left\lfloor \frac{2v - bk}{b} \right\rfloor \qquad k' \leq k_0 = k - n_0$$


A_1
A_n
3
B_1
B_n
A
B
4
1
2
7
8
6
D
C
D_1
D_n
5
C_1
C_n



The drones contribute nothing to the number of spanning trees.



The drones contribute nothing to the number of spanning trees.
$\tilde{R}_{A_1C_1} = 1 + \tilde{R}_{AC} + 1.$

Sum of the pairwise resistances

Theorem (cf. Herzberg and Jarrett, 2007)

If there are n drones in each block of Δ,
and the core design Γ has v' treatments in b blocks of size k'
then the sum of the treatment resistances in Δ

$$= bn(bn + v' - 1) + R_T(\Gamma) + nR_{BT}(\Gamma) + n^2 R_B(\Gamma),$$

where

$$\begin{aligned} R_T(\Gamma) &= \text{the sum of the treatment resistances in } \Gamma \\ R_B(\Gamma) &= \text{the sum of the block resistances in } \Gamma \\ R_{BT}(\Gamma) &= \text{the sum of the treatment-block resistances in } \Gamma. \end{aligned}$$

Consequences

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2. If v is large then n is large,
   so we need to focus on reducing $R_B(\Gamma)$,
   so it may be best to increase the number of drones
   and decrease k' (the size of blocks in the core design Γ),
   so that average replication within Γ is more than 2.

An example of this non-intuitive result

If there are $4(2+n)$ varieties in 4 blocks of size $4+n$, the design on the left is A-better than the design on the right if and only if $n < 50$.

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

1	2	3	$n+1$ drones
1	2	4	$n+1$ drones
1	3	4	$n+1$ drones
2	3	4	$n+1$ drones

Conjectures

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

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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.

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Within the last nine months, three collaborators contacted me by email to say something like

> *You might be interested in this optimal design that my computer found.*

Motivation: IIb

In one case, I replied

Here is a better design than yours. It is not equi-replicate.

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Third case: similar.

If someone can find a function $f(v, b, k)$ and
a criterion on its value such that, when the criterion is satisfied, programs should relax their usual assumptions in their search for good experimental designs, it would be immensely useful.

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