Graphs from block designs: concurrence, distance, variance and electrical resistance

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Combinatorics 2008

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- The combinatorialist's points are the statistician's treatments.
- Blocks are more-or-less the same to both, except that the statistician can allow a treatment to occur on more than one unit in a block.
- With this proviso, the statistician's experimental units are the combinatorialist's flags.

Microarray experiments

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$$v \text{ treatments} \longrightarrow v \text{ vertices}$$
$$b \text{ blocks} \longrightarrow b \text{ edges}$$

Biologists versus mathematicians: Designs for 6 treatments

12 blocks (edges)

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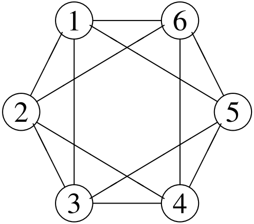

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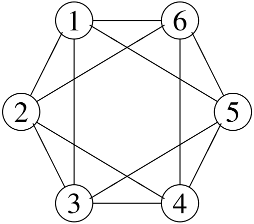

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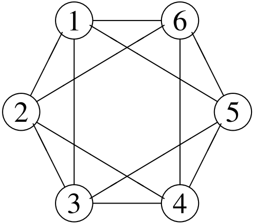

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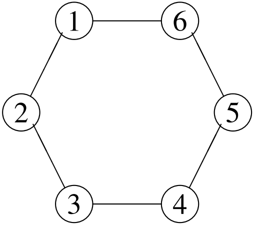

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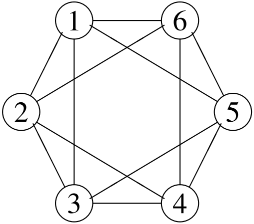

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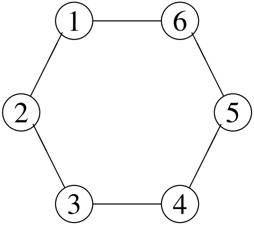

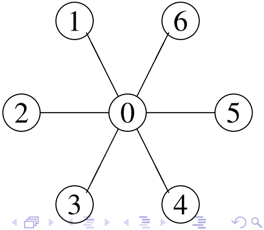

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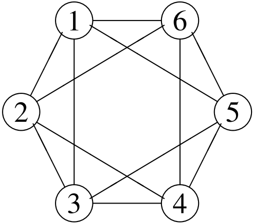

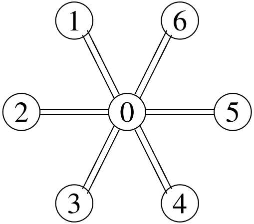

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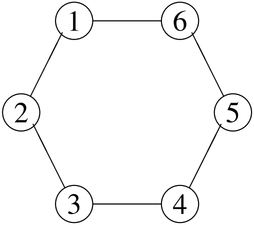

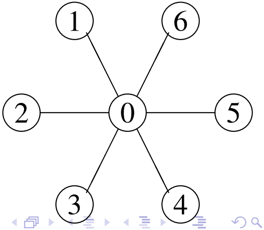

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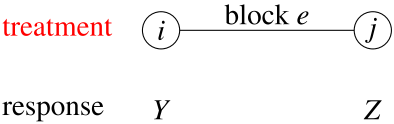
2. We need to optimize a single summary measure (coming up later).
3. We want it to remain good if we lose a few observations (even later).

Estimation and variance



Estimation and variance

treatment 

response Y Z

$$\begin{aligned} \text{Assume that } Y &= \tau_i + \beta_e + \text{noise} \\ Z &= \tau_j + \beta_e + \text{other noise} \end{aligned}$$

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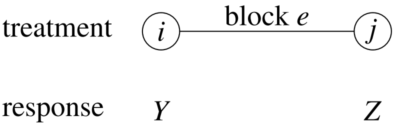

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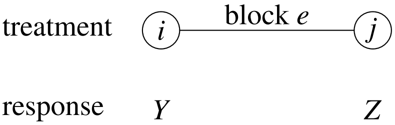

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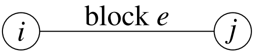

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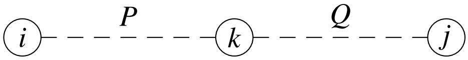
Put $V_{ij} =$ variance of the estimator for $\tau_i - \tau_j$ using the whole graph.

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

Variance: series



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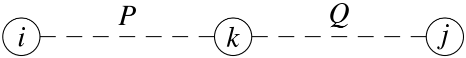

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\begin{aligned}
P &= \text{estimator for } \tau_i - \tau_k \text{ with variance } d \\
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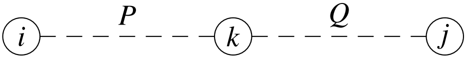

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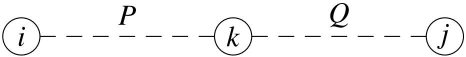

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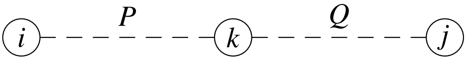

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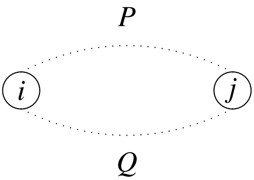

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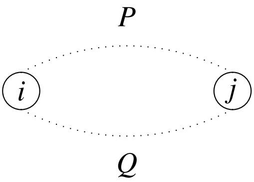

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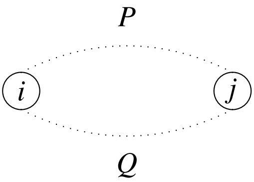

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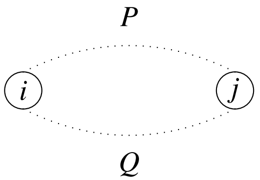

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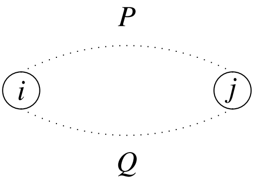

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Eureka!

Variance is the same as resistance!

(if the block size is 2)

$$\begin{aligned}\text{Block design} &\longrightarrow \text{(multi-)graph}\\ &\longrightarrow \text{electrical network with resistance 2 in each edge}\end{aligned}$$

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(Good for sparse graphs with many vertices of valency 2.)

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Theorem

$$V_{ij} = 2 \times \frac{\textit{number of spanning thickets with i, j in different parts}}{\textit{number of spanning trees}}$$

Conjecture relating variance to distance

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If the distance in the graph between vertices i and j is less than the distance between k and l then $V_{ij} \leq V_{kl}$.

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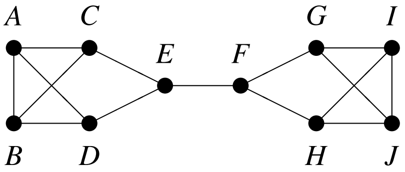

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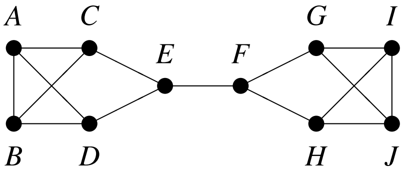

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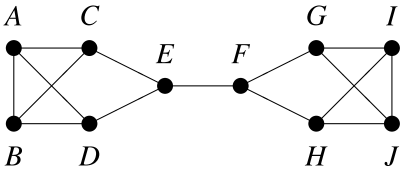

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... but that is a terrible block design!

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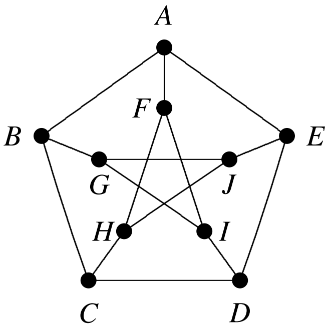

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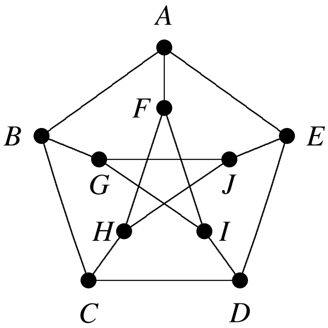

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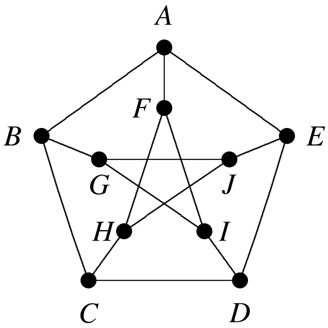

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The second graph is strongly regular.

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Proof use the fact that L^- is in the Bose-Mesner algebra of the graph.

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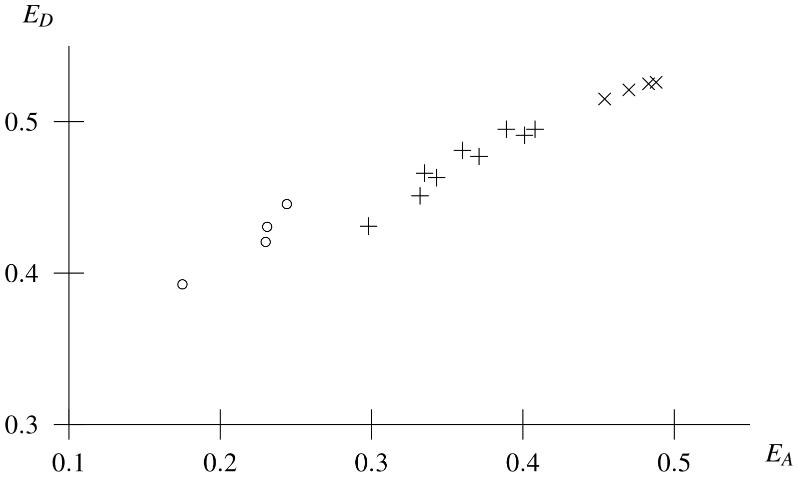
The D and A criteria for all regular graphs with 8 vertices and valency 3



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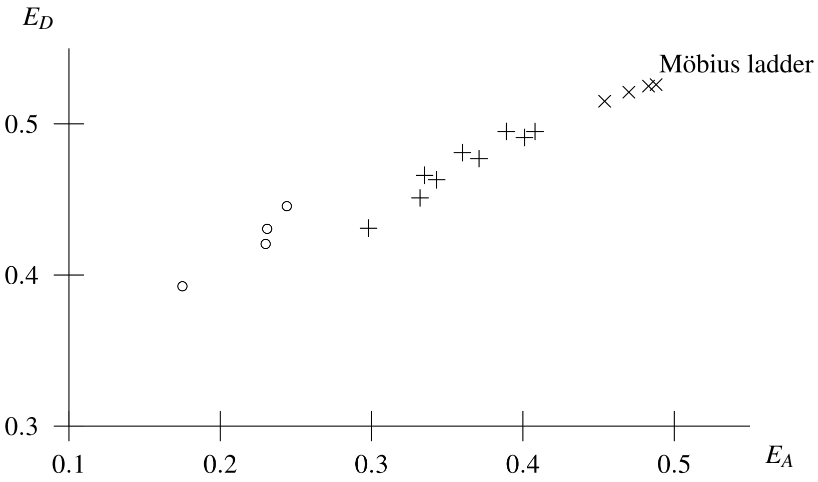

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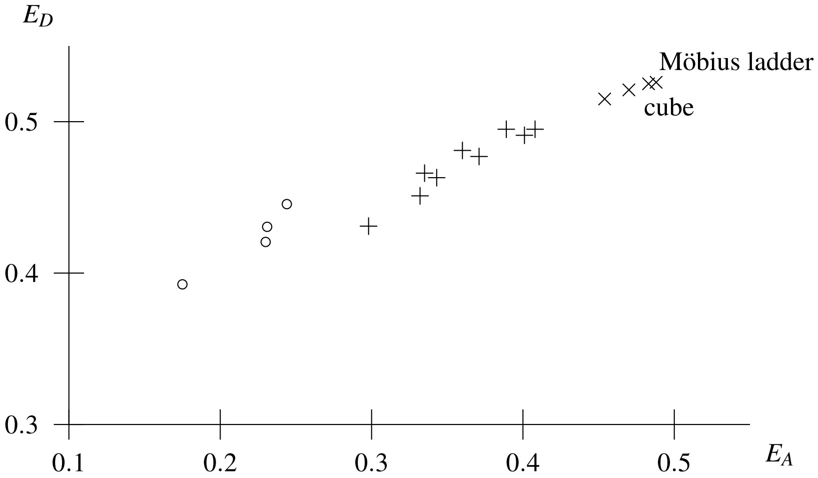

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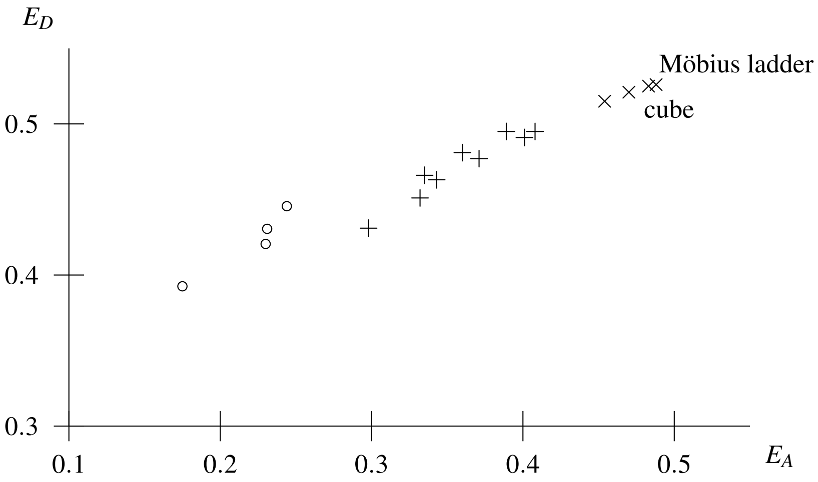


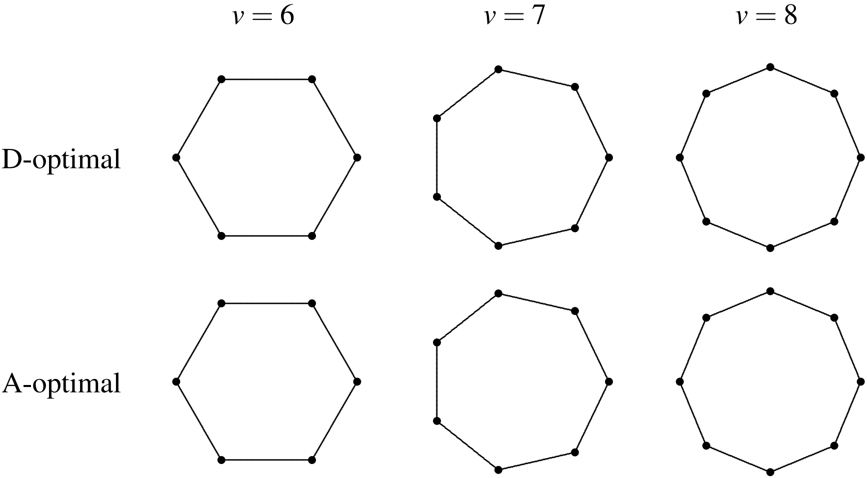
Robustness: edge-connectivity 3, 2, 1 shown as $\times$, $+$, $\circ$ respectively.

Some history: what happens when $b = v$?

Computer investigation by

- Jones and Eccleston (1980)
- Kerr and Churchill (2001)
- Wit, Nobile and Khanin (2005)
- Ceraudo (2006).

Optimal designs when $b = v$



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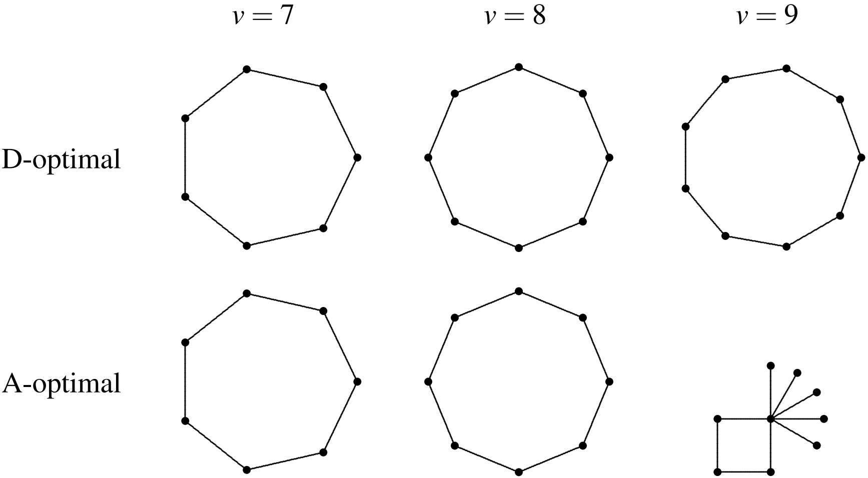

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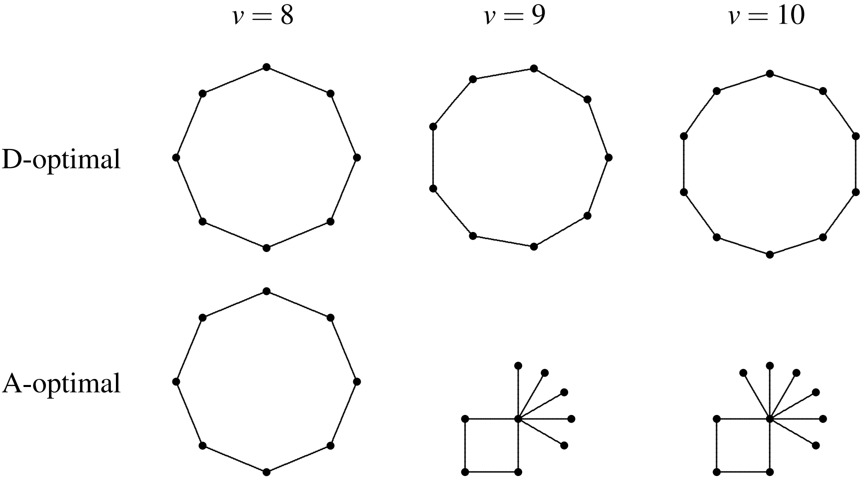

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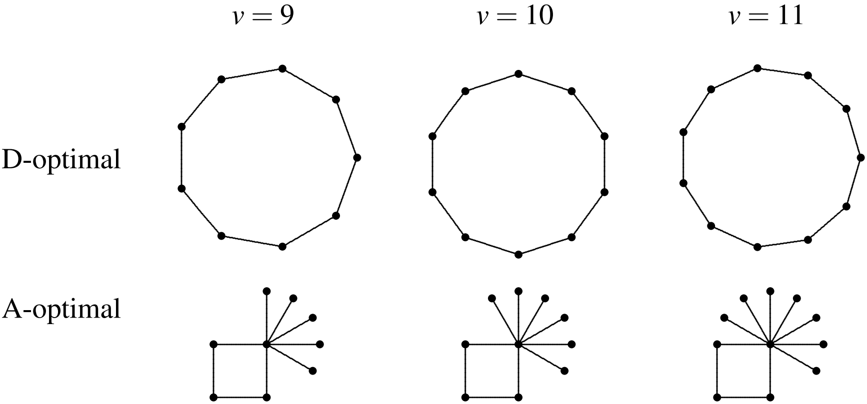

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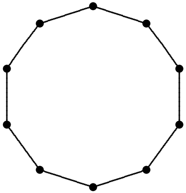
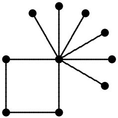


10 spanning trees



4 spanning trees

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

Results about A-optimality

Theorem (Thanks to Emil Vaughan)

$$\sum_{i<j} V_{ij} = 2 \times \frac{\sum_{\text{thickets } F} |F_1|\,|F_2|}{\textit{number of spanning trees}}$$

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The A-optimal design with $b = v$ is

- *the loop design (single circuit) if $v \leq 8$;*
- *a star glued to a quadrilateral if $9 \leq v \leq 11$;*
- *a star glued to a quadrilateral or a triangle if $v = 12$;*
- *a star glued to a triangle if $v \geq 13$.*

What happens when $b = v + 1$?

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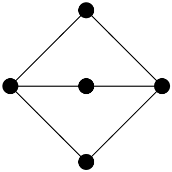

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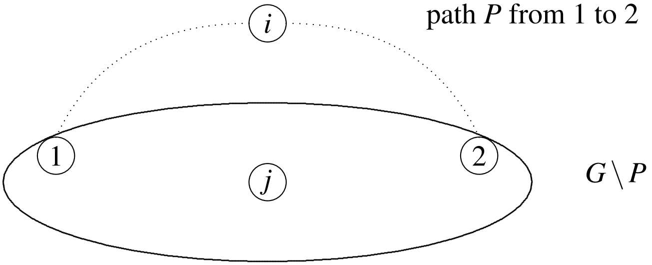
D-optimal designs do not have leaves.

Proof outline



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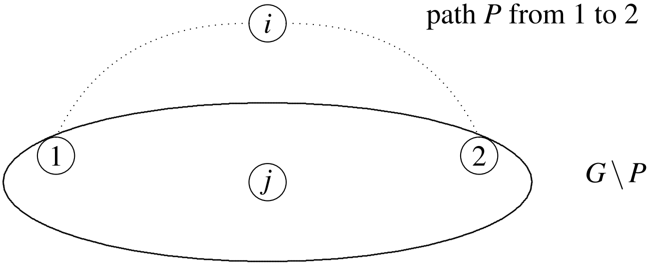

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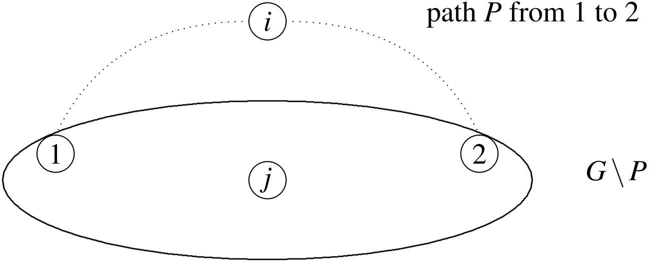

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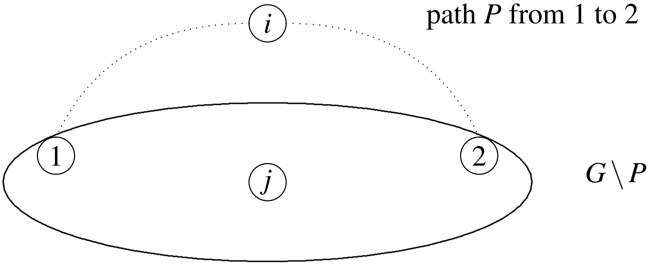

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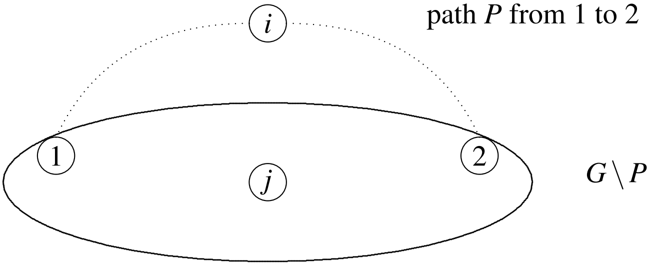

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Fix $b/v = c$. In a regular graph with valency $2c$, many(?) variances will probably(?) increase unboundedly as v increases.

In $cK_{1,v}$, all the variances are $2/c$ or $4/c$.

There are probably(?) more spanning trees in regular graphs than in multi-stars.

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But $d_i = \sum_j a_{ij} = r_i(k-1)$, so $D = (k-1)R$ and

$$L = R - \frac{(R+A)}{k} = \frac{(k-1)R - A}{k} = \frac{D-A}{k} = \frac{\text{Laplacian matrix}}{k}.$$

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Theorem

If the concurrence graph is a multiple of the complete graph K_v, then the design is optimal on all criteria.

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- Do the answers to the above questions change if we restrict to graphs that are 'near-optimal'?

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