Conflicts between optimality criteria for block designs with low replication

R. A. Bailey

Queen Mary University of London

r.a.bailey@qmul.ac.uk

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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?

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.

Design $\rightarrow$ 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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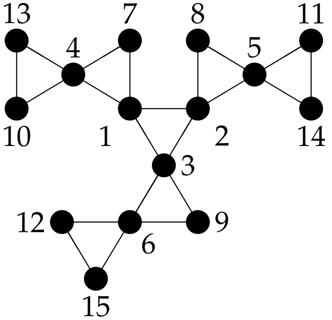

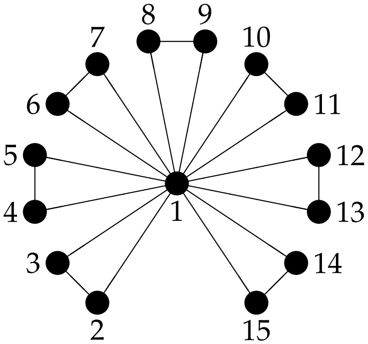

Graph $\to$ matrix

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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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

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

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

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- 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

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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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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 $1/I$.

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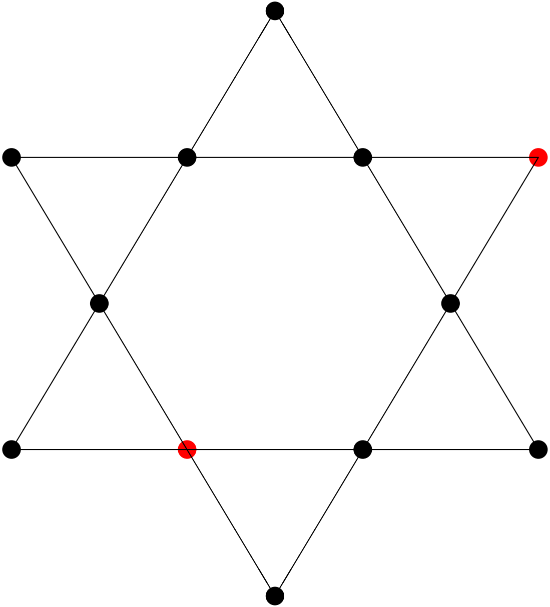
Effective resistances are easy to calculate without matrix inversion if the graph is sparse.

Example calculation



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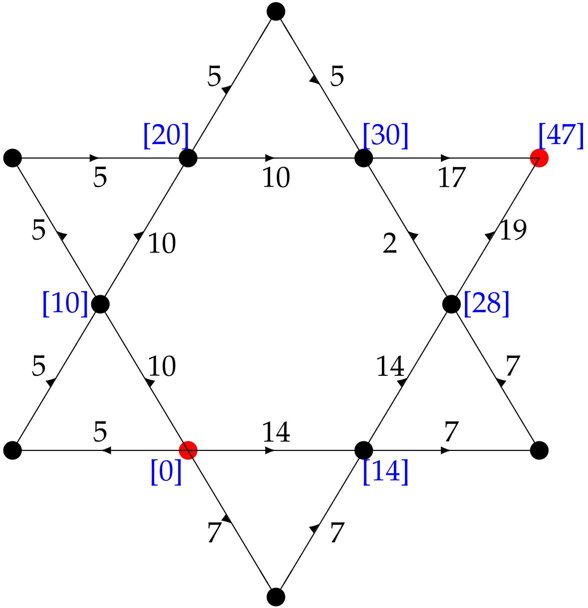

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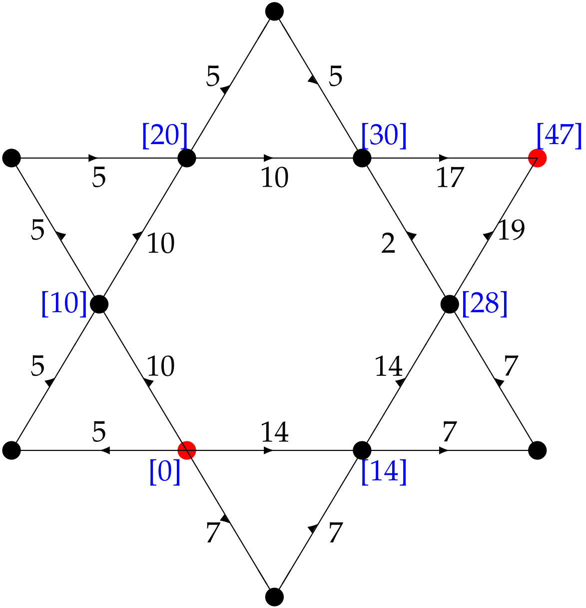

$V = 47$

$I = 36$

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

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

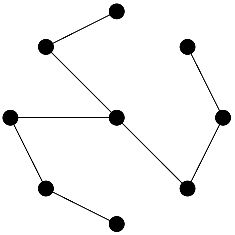
$$\theta_1 \leq c \left(\frac{1}{m} + \frac{1}{n} \right).$$

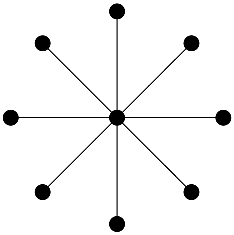
If c is small but m and n are both large, then θ_1 is small.

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





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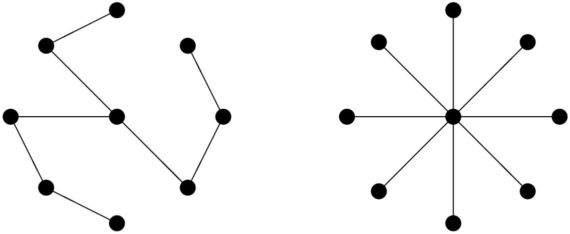

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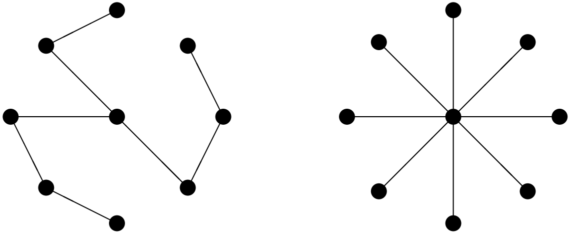
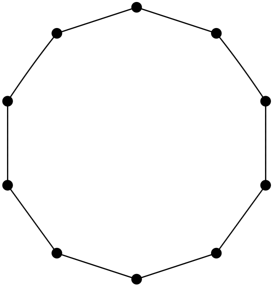


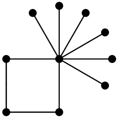
The D-criterion does not differentiate them.

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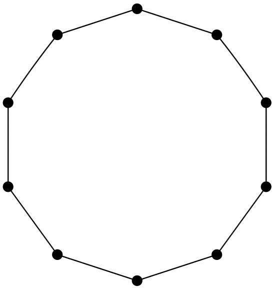
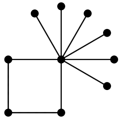
If $k = 2$ and $b = v$ then the design consists of a cycle with trees attached to some vertices.

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





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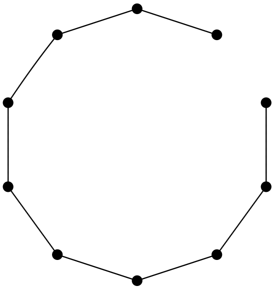

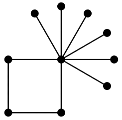

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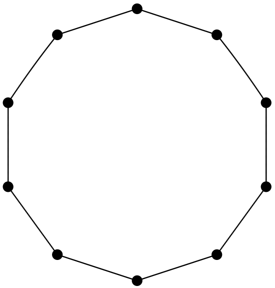

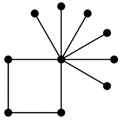

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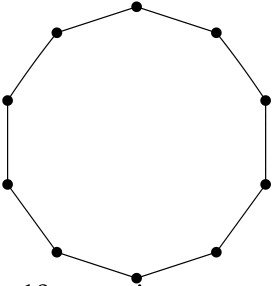
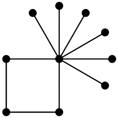


10 spanning trees



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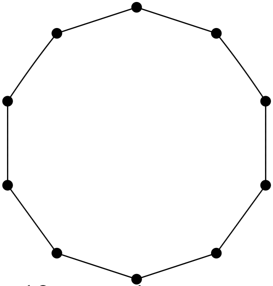

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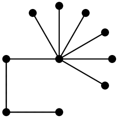

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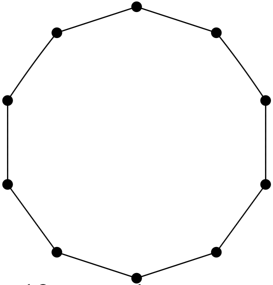

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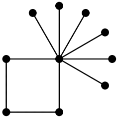

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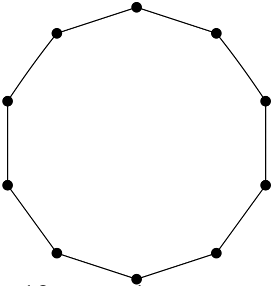

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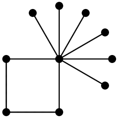
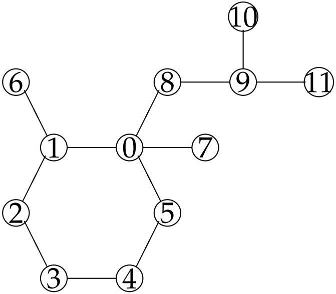
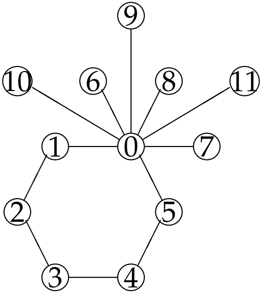


4 spanning trees

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 $v \leq 6$
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The A-optimal designs and E-optimal designs are far from equi-replicate.
The change is sudden, not gradual.

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

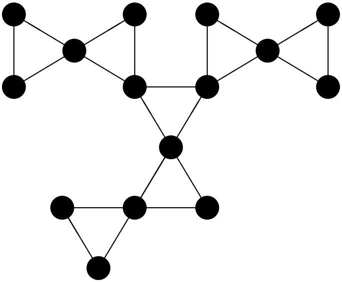
"It seems to be just block size 2 *that is a problem."*

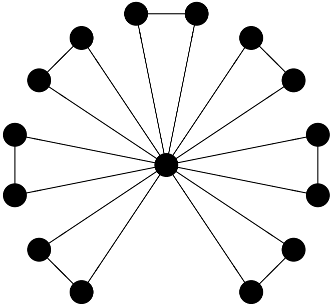
Block size 3, but minimal b

The remaining arguments extend easily to general block size.

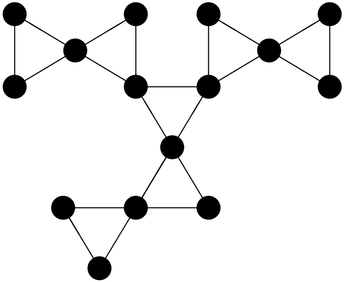
When $k = 3$, for a connected design, we need $2b \geq v - 1$.

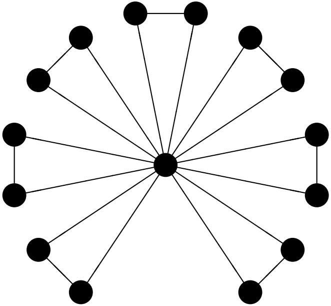
If $2b + 1 = v$ then all designs are gum-trees,
in the sense that there is a unique sequence of blocks
from any one treatment to another.





Block size 3, but minimal b: D





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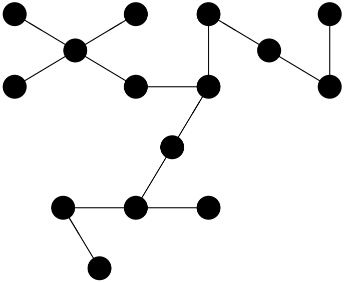

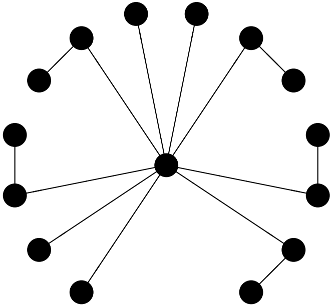

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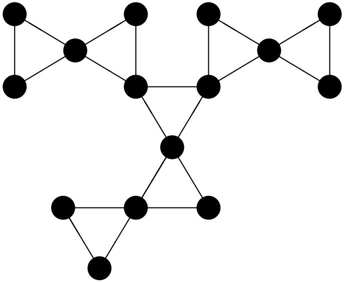
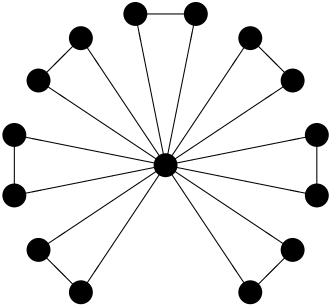


3^7 spanning trees



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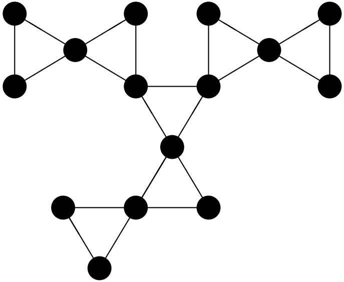

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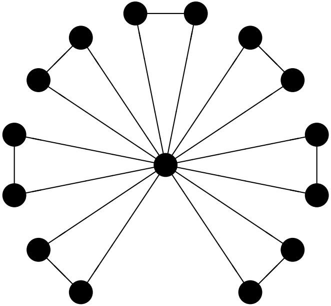
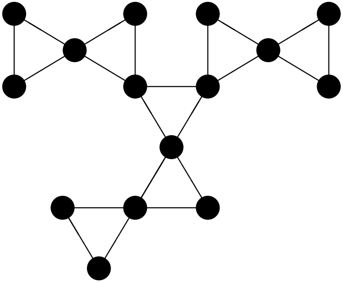
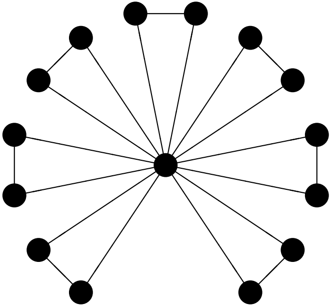


3^7 spanning trees

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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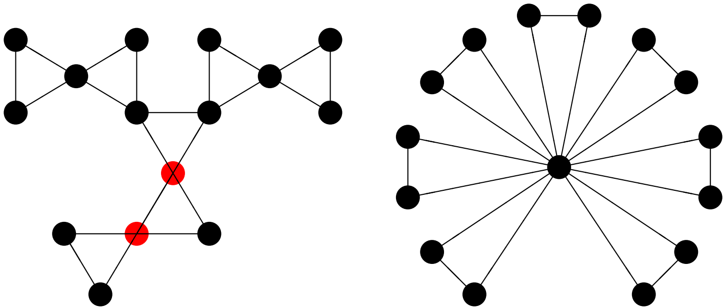

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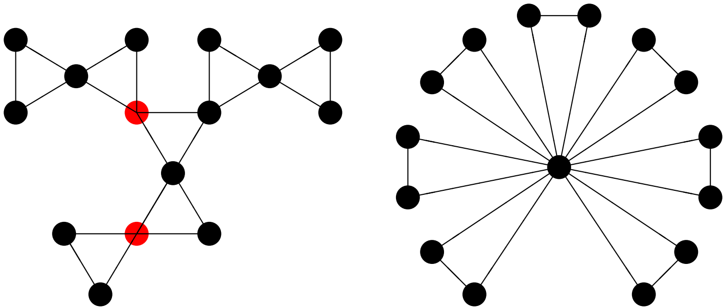
If $i, j \in$ same block then $R_{ij} = \frac{2}{3}$.

Block size 3, but minimal b: A



Let R_{ij} be the effective resistance between treatments i and j.
If $i, j \in$ same block then $R_{ij} = \frac{2}{3}$.
If $i, j \in$ distinct intersecting blocks then $R_{ij} = \frac{2}{3} + \frac{2}{3} = \frac{4}{3}$.

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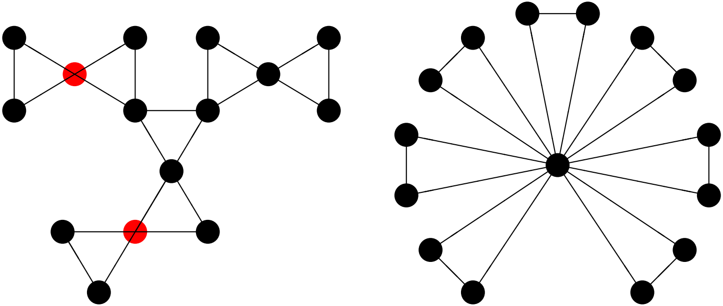

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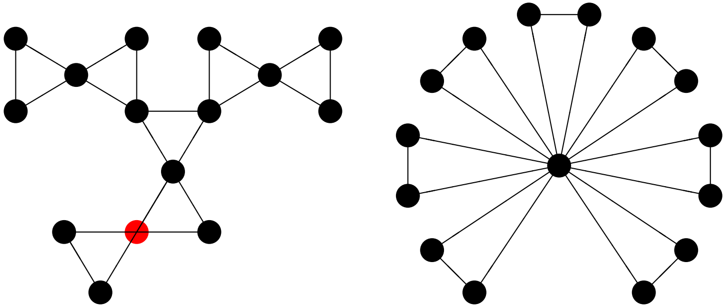

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The only A-optimal designs are the queen-bee designs.

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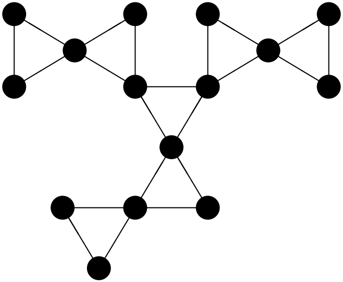

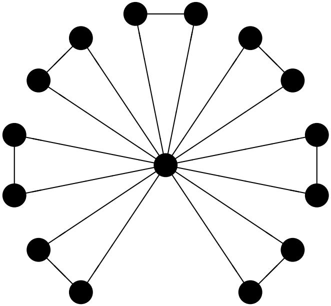

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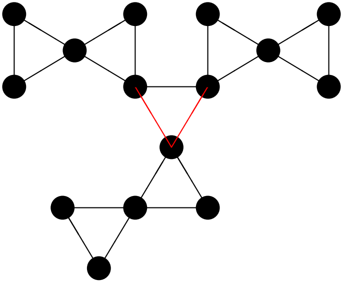

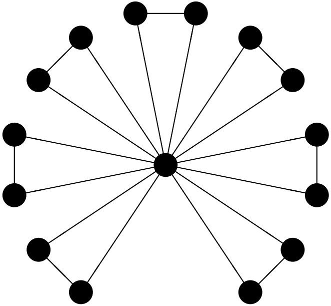

$$\theta_1 \leq 2\left(\frac{1}{5} + \frac{1}{10}\right)$$

$$\theta_1 \geq 1$$

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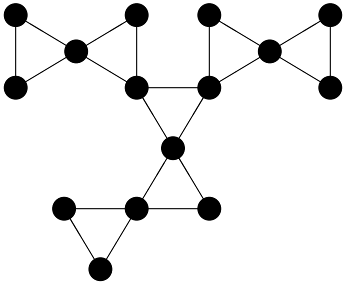

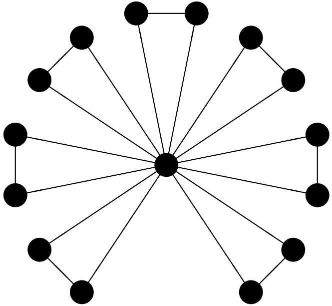

$\theta_1 \leq 2\left(\frac{1}{5} + \frac{1}{10}\right)$

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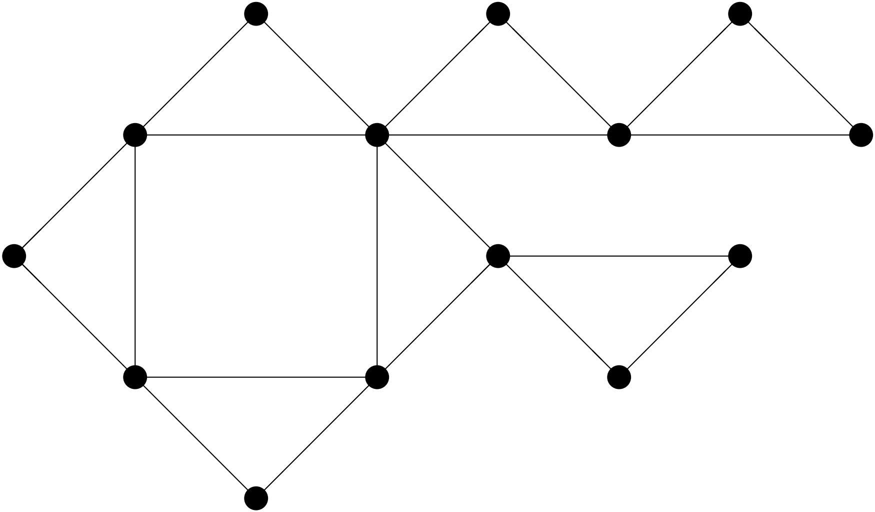
The only E-optimal designs are the queen-bee designs.

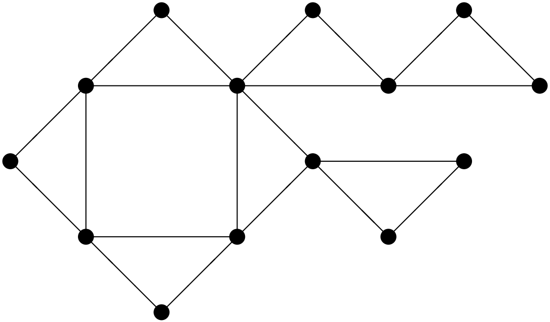
Block size 3, but $b =$ minimal $+1$

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.



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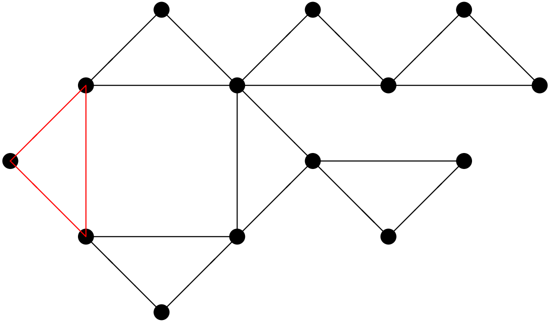

For a spanning tree:
choose a block in the gum-cycle s

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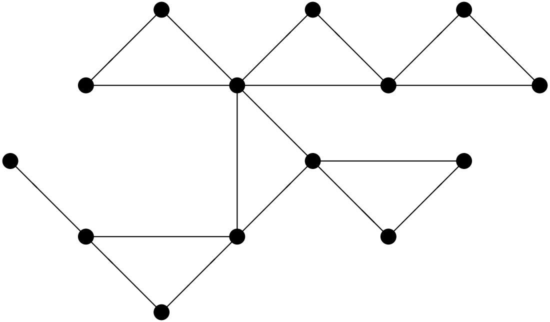

For a spanning tree:

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

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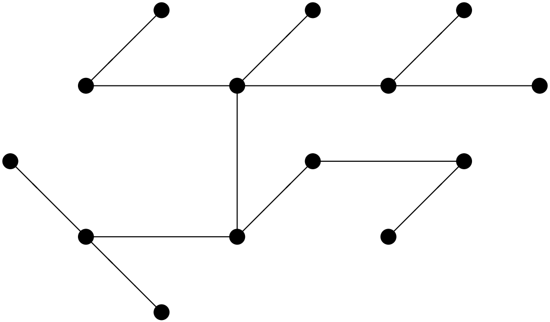

For a spanning tree:

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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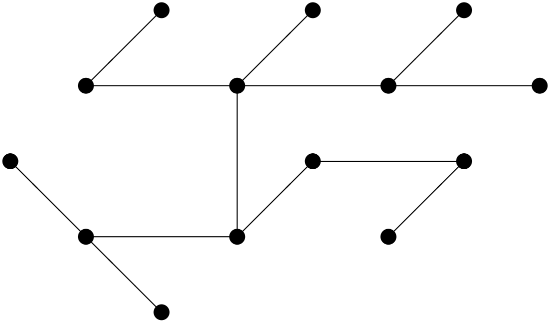

For a spanning tree:

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.

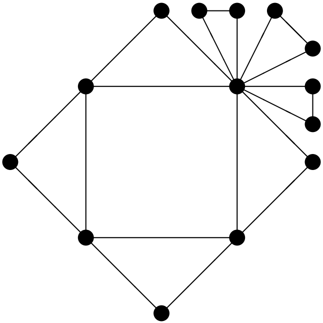
If $v = b(k-1)$ then the only D-optimal designs are the gum-cycles.

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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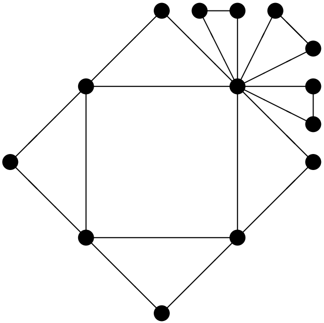

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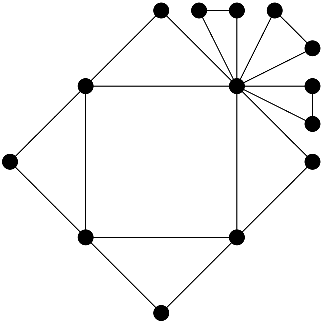

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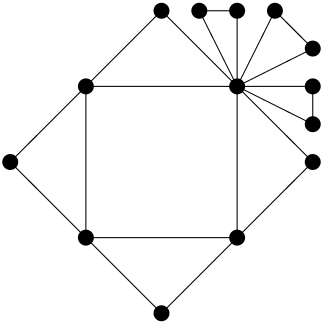

The sum of pairwise effective resistances is a cubic function of s.

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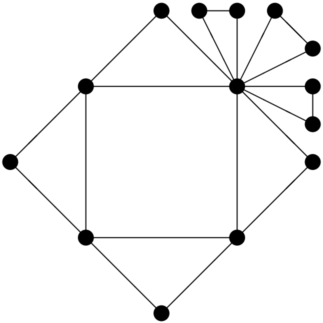

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A-optimal designs do not have s large.

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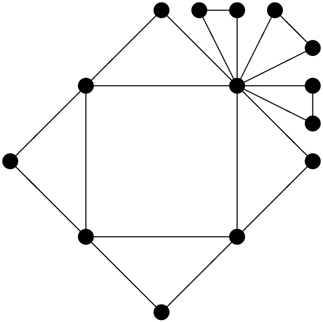

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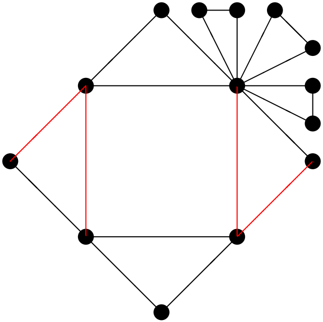

If s is large then there is a cutset of size 4 with two large parts.

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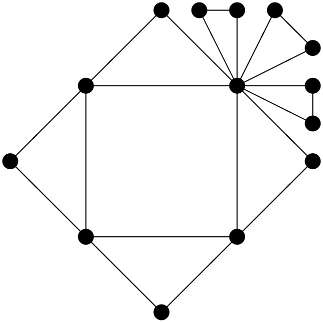

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New asymptotic results (large v)

Current work by J. Robert Johnson and Mark Walters.

Block size 2;

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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)

Large blocks; many unreplicated treatments

The milling phase of a wheat variety trial has 224 varieties in 14 blocks of size 20.

Large blocks; many unreplicated treatments

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($280 - 224 = 56$ and $224 - 56 = 168$,
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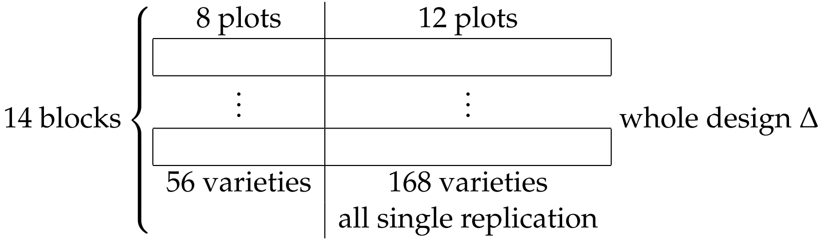

Subdesign Γ has 56 varieties
in 14 blocks of size 8.

Remember that average replication is very low

Yates (1936) concluded that square-lattice incomplete-block designs are superior to the inclusion of controls, but all of his examples had average replication equal to three or more.

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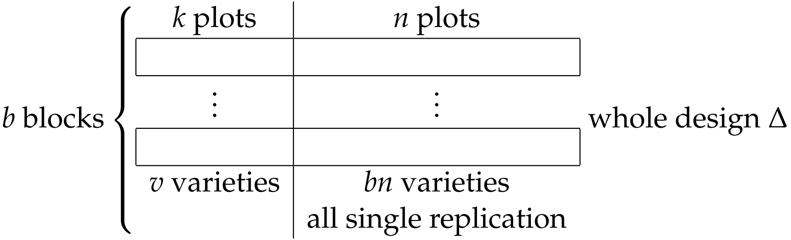
Yates (1936) concluded that square-lattice incomplete-block designs are superior to the inclusion of controls, but all of his examples had average replication equal to three or more.

Here we assume that average replication is (much) less than two.

A general block design with average replication less than 2



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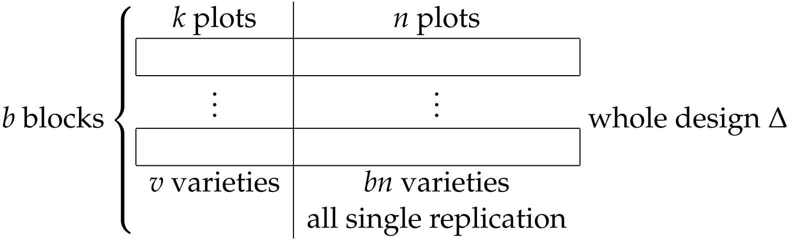
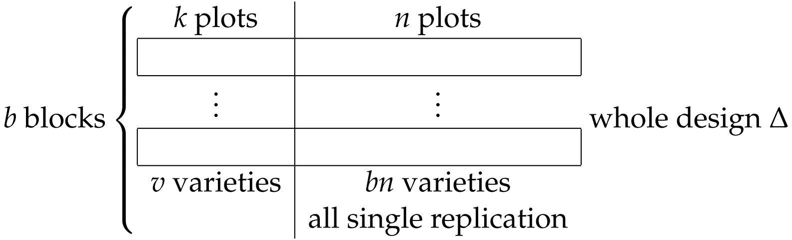


Whole design Δ has $v + bn$ varieties in b blocks of size $k + n$;

A general block design with average replication less than 2



Whole design Δ has $v + bn$ varieties in b blocks of size $k + n$;
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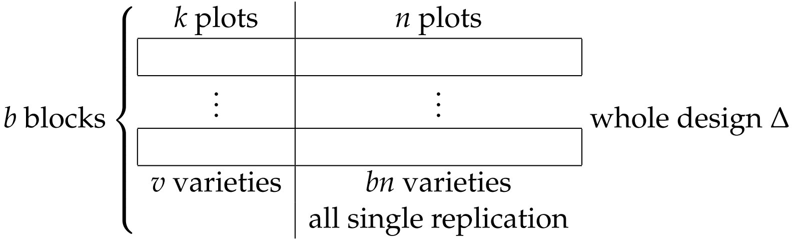
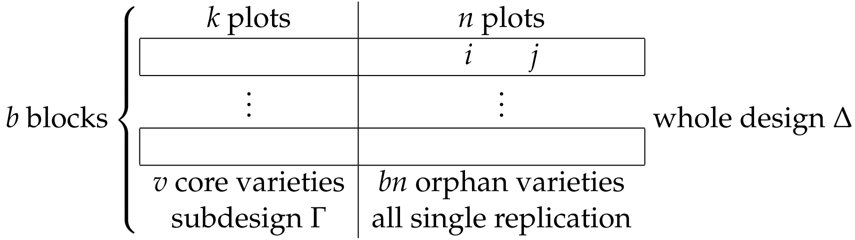
A general block design with average replication less than 2



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

Pairwise variance: two orphans in the same block



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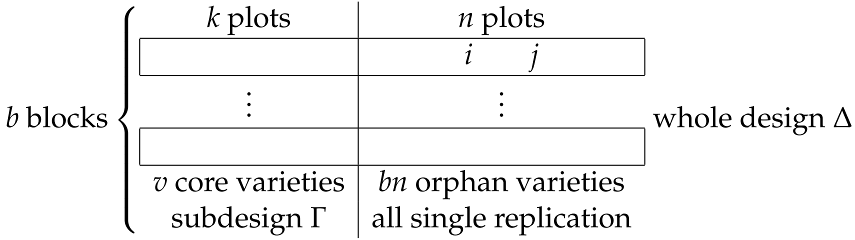
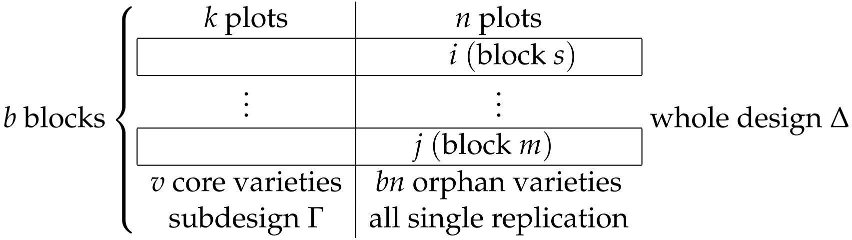


$$\mathrm{Var}_{\Delta}(\hat{\tau}_i - \hat{\tau}_j) = 2\sigma^2.$$

Pairwise variance: two orphans in different blocks

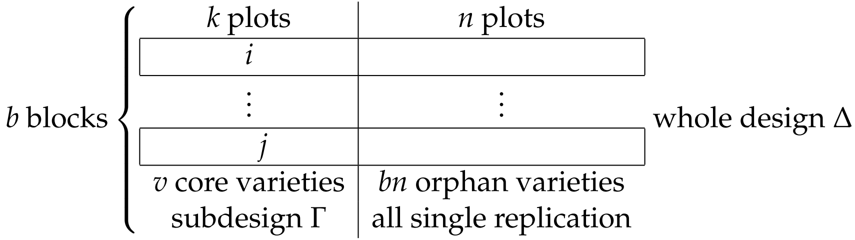


Pairwise variance: two orphans in different blocks

	k plots	n plots	
b blocks		i (block s)	whole design Δ
	$\vdots$	$\vdots$	
		j (block m)	
	v core varieties subdesign Γ	bn orphan varieties all single replication	

$$\mathrm{Var}_\Delta(\hat{\tau}_i - \hat{\tau}_j) = 2\sigma^2 + \mathrm{Var}_\Gamma(\hat{\beta}_s - \hat{\beta}_m).$$

Pairwise variance: two core varieties



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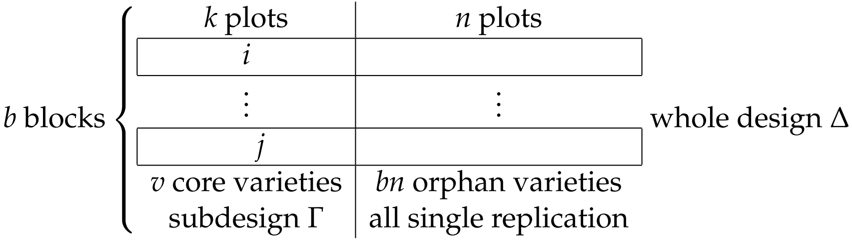
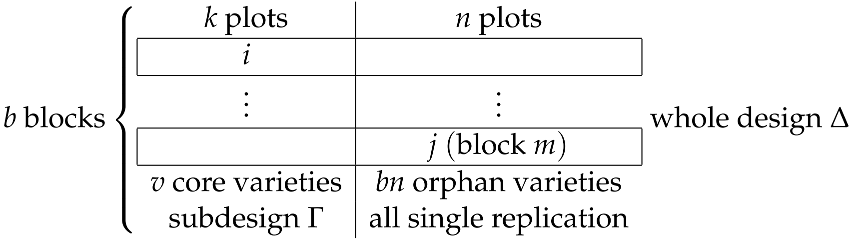


$$\mathrm{Var}_{\Delta}(\hat{\tau}_i - \hat{\tau}_j) = \mathrm{Var}_{\Gamma}(\hat{\tau}_i - \hat{\tau}_j).$$

Pairwise variance: one core variety and one orphan



Pairwise variance: one core variety and one orphan

	k plots	n plots	
b blocks	i		whole design Δ
	$\vdots$	$\vdots$	
		j (block m)	
	v core varieties subdesign Γ	bn orphan varieties all single replication	

$$\mathrm{Var}_{\Delta}(\hat{\tau}_i - \hat{\tau}_j) = \sigma^2 + \mathrm{Var}_{\Gamma}(\hat{\tau}_i + \hat{\beta}_m).$$

Sum of the pairwise variances

Theorem (cf Herzberg and Jarrett, 2007)

The sum of the variances of treatment differences in Δ

$$= constant + V_1 + nV_3 + n^2 V_2,$$

where

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

(If Γ is equi-replicate then V_2 and V_3 are both increasing functions of V_1.)

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Theorem (cf Herzberg and Jarrett, 2007)

The sum of the variances of treatment differences in Δ

$$= constant + V_1 + nV_3 + n^2 V_2,$$

where

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

(If Γ is equi-replicate then V_2 and V_3 are both increasing functions of V_1.)

Consequence

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

A less obvious consequence

Consequence

If n or b is large,
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.

$5n + 10$ treatments in 5 blocks of size $4 + n$

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

Youden and Connor (1953): "experiments in physics do not need much replication because results are not very variable" —introduced chain block designs

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subdesign is dual of BIBD (Herzberg and Andrews, 1978)

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best subdesign for $k = 4$

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best subdesign for $k = 3$ is better for large n if $b \neq 5$

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5	1	2	0	E_1	$\cdots$	E_n

best subdesign for $k = 3$ is better for large n if $b \neq 5$

K_1	K_2	1	2	A_1	$\cdots$	A_n
K_1	K_2	3	4	B_1	$\cdots$	B_n
K_1	K_2	5	6	C_1	$\cdots$	C_n
K_1	K_2	7	8	D_1	$\cdots$	D_n
K_1	K_2	9	0	E_1	$\cdots$	E_n

better for large n if $b > 13$ even if there is no interest in controls

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