Optimal design of experiments with very low average replication

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Motivation

Poster at LinStat 2010, Tomar, Portugal, July 2010:
'Unreplicated experiments in early stage breeding programs'
by Katarzyna Marczyńska and Stanisław Mejza.

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Question from Brian Cullis and David Butler, Adelaide, Australia, November 2010:
If we are not interested in control treatments, we know that we can get more information by replacing the check plots by second replicates of some treatments—can you prove this?

Abstract

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I shall compare designs under the A criterion when the average replication is much less than two.

Agricultural plant-breeding trials

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How do you design the experiment?

Assume that

$$\text{number of varieties} < \text{number of plots}$$

and

$$\text{number of plots} << 2 \times (\text{number of varieties}).$$

Some notation

$$f(\omega) = \text{variety on plot } \omega.$$

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Assume that

$$Y_\omega = \tau_{f(\omega)} + \text{stuff depending on plots.}$$

We want to minimize

$$\sum_i \sum_{j \neq i} \text{Var}(\hat{\tau}_i - \hat{\tau}_j).$$

Simplest model

$$Y_\omega = \tau_{f(\omega)} + \epsilon_\omega$$

where

$$\mathbb{E}(\epsilon_\omega) = 0, \qquad \mathrm{Var}(\epsilon_\omega) = \sigma^2,$$

$$\text{and} \quad \mathrm{Cov}(\epsilon_\omega, \epsilon_{\omega'}) = 0 \quad \text{if } \omega \neq \omega'.$$

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The A-optimal design has
2 plots for some varieties and 1 plot for all other varieties,
and is completely randomized.

Simplest model: example

56 varieties have replication 2;

168 varieties have replication 1.

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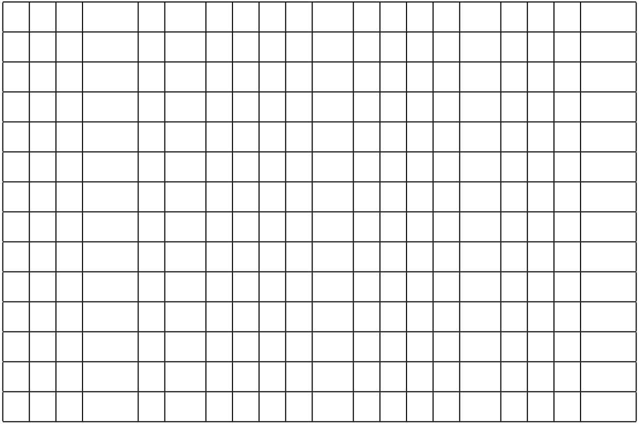

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															1				
			2																
					1														
										2									

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															1				
			2																
																			57
					1														
			58																
									2										

A breeder says . . .

Unfair!

The single plot with my variety was in an infertile part of the field.

Fixed spatial trend

$$Y_\omega = \tau_{f(\omega)} + g(\omega) + \epsilon_\omega$$

where

$$g(\omega) \text{ is a two-dimensional low-degree polynomial in } \omega,$$

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use one plot for each new variety
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place the "control" plots in a grid;
use the "control" responses to estimate the polynomial trend;
estimate each variety effect by subtracting the trend value from its response.

Spatial trend: example

56 plots for “control”

224 new varieties have replication 1.

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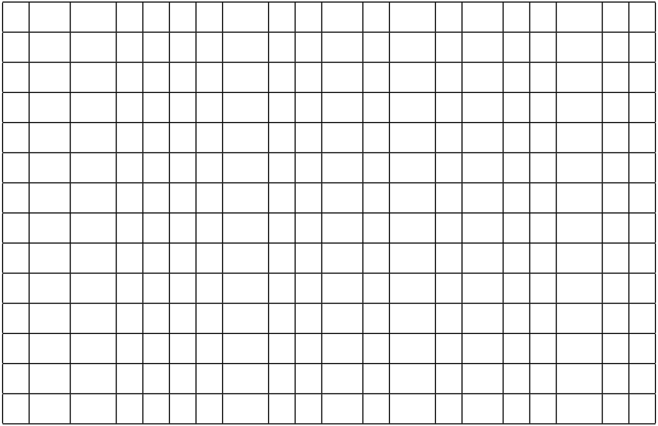

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		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		

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		X					X					X					X		
		X					X			3		X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
	2	X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
		X					X					X		1			X		
		X					X					X					X		
		X					X					X					X		
		X					X					X					X		
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		X					**X**					**X**					**X**		
		X					**X**			**3**		**X**					**X**		
		X					**X**					**X**					**X**		
		X					**X**					**X**					**X**		
		X					**X**					**X**					**X**		
	2	**X**					**X**					**X**					**X**		
		X					**X**					**X**					**X**		
		X					**X**					**X**					**X**		
		X					**X**					**X**					**X**		
		X					**X**					**X**		**1**			**X**		
		X					**X**					**X**					**X**		
		X					**X**					**X**					**X**		
		X					**X**					**X**					**X**		
		X					**X**					**X**					**X**		

Controls are on every fifth plot, working along rows.

Spatial trend: example, another layout

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	X							X			X							X	
				X	X									X	X				
X									X	X									X
			X			X							X			X			
		X					X					X					X		
	X							X			X							X	
				X	X									X	X				
X									X	X									X
			X			X							X			X			
		X					X					X					X		
	X							X			X							X	
				X	X									X	X				
X									X	X									X
			X			X							X			X			

Controls are on every 5th plot, working boustrophedon along columns.

Spatial trend: example, a third layout

56 plots for "control"

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Spatial trend: example, a third layout

56 plots for "control"

224 new varieties have replication 1.

	X		X			X		X			X		X			X		X	
	X		X			X		X			X		X			X		X	
	X		X			X		X			X		X			X		X	
	X		X			X		X			X		X			X		X	
	X		X			X		X			X		X			X		X	
	X		X			X		X			X		X			X		X	
	X		X			X		X			X		X			X		X	

Controls are on a complete sub-rectangle.

Spatial trend: example, what should we optimize?

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X	X				X	X							X	X				X	X
X	X				X	X							X	X				X	X
X	X																	X	X
X	X				X									X				X	X
									X	X									
									X	X									
X	X				X									X				X	X
X	X																	X	X
X	X				X	X							X	X				X	X
X	X				X	X							X	X				X	X

Controls are positioned to make the average variance of prediction small if the trend is a polynomial of degree three.

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X	X	X															X	X	X
X																			X
X																			X
X									X	X									X
X									X	X									X
X									X	X									X
X									X	X									X
X																			X
X																			X
X	X	X															X	X	X
X	X	X						X	X	X	X						X	X	X

Controls are positioned to make the maximum variance of prediction small if the trend is a polynomial of degree two.

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If the plots are not square, do the optimal designs change?

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Yates (1936), Atiqullah and Cox (1962) consider controls spread throughout the field. In their analysis, a weighted mean of the response on the nearest controls is used as a covariate, rather than being simply subtracted.

This is a rather different model.

Spatial correlation

$$Y_\omega = \tau_{f(\omega)} + \epsilon_\omega$$

where

$$\mathbb{E}(\epsilon_\omega) = 0, \qquad \mathrm{Var}(\epsilon_\omega) = \sigma^2,$$

and

$\mathrm{Cov}(\epsilon_\omega, \epsilon_{\omega'})$ depends on the spatial relationship between ω and ω'.

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Blocks

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(One block has all the stony plots;
one block has all the plots near the trees;
one block has all the plots near the rabbit warren, ...)

$$Y_\omega = \tau_{f(\omega)} + \beta_{h(\omega)} + \epsilon_\omega$$

where

$$h(\omega) = \text{block containing } \omega,$$

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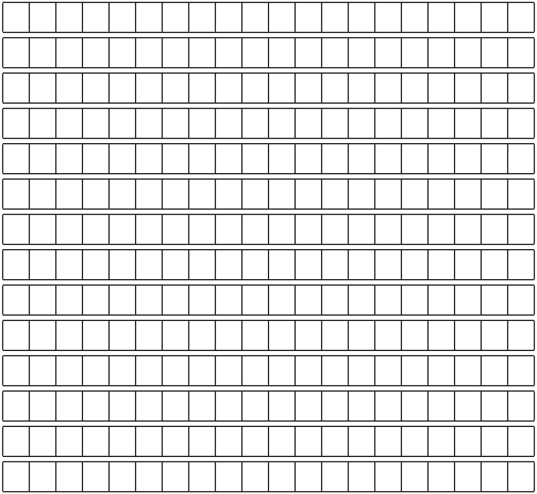
Blocks: example

Rows are blocks, so there are 14 blocks, each with 20 plots.



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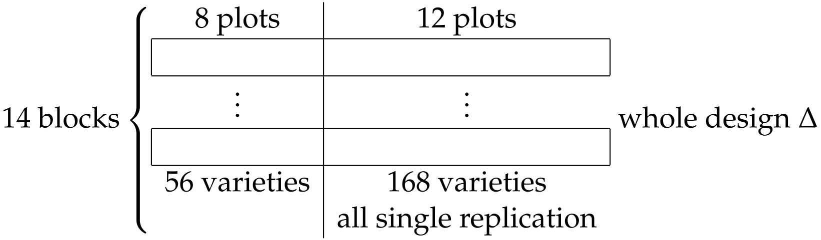

Subdesign Γ has 56 varieties
in 14 blocks of size 8.

Blocks: remember that replication is very low

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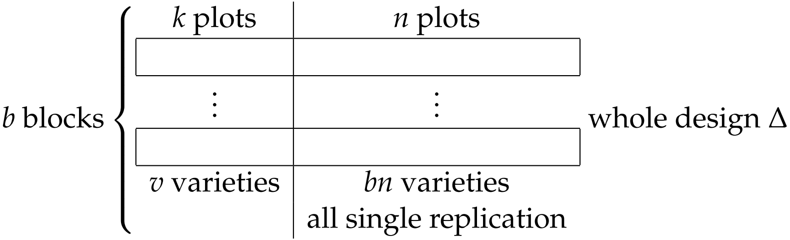
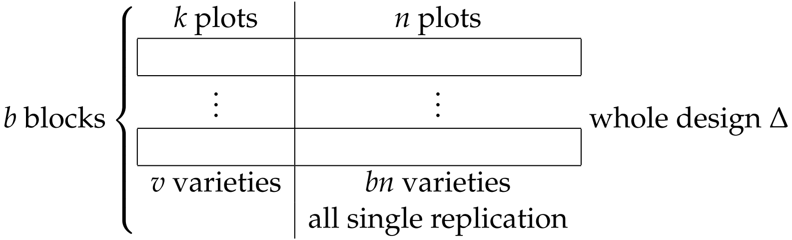
Yates (1936) concluded that square-lattice incomplete-block designs are superior to the inclusion of controls, but all of his examples had average replication equal to three or more.

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

A general block design with average replication less than 2



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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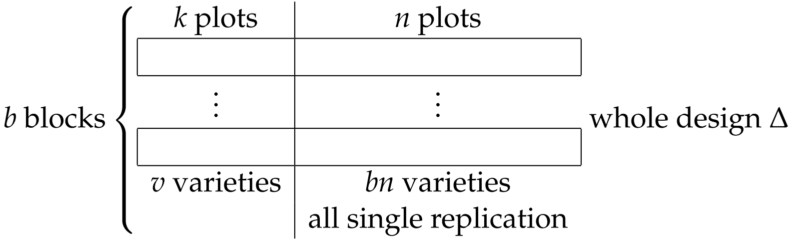

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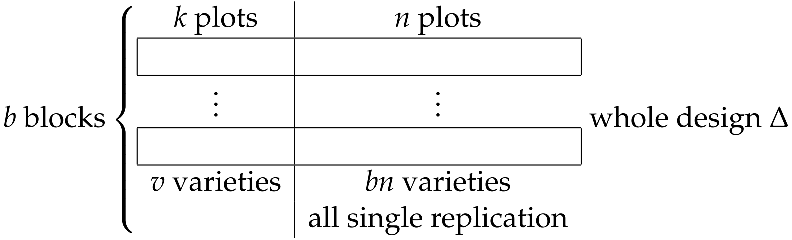
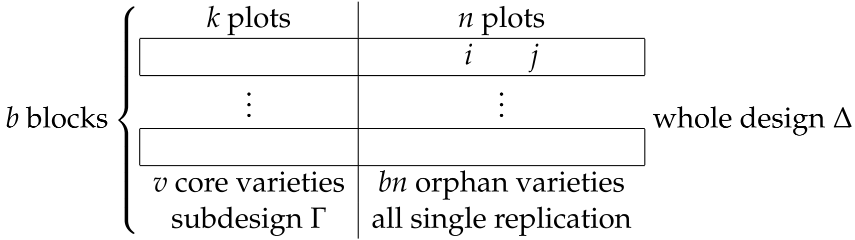


Whole design Δ has $v + bn$ varieties in b blocks of size $k + n$;
the subdesign Γ has v core varieties in b blocks of size k;
call the remaining varieties orphans.

Pairwise variance: two orphans in the same block



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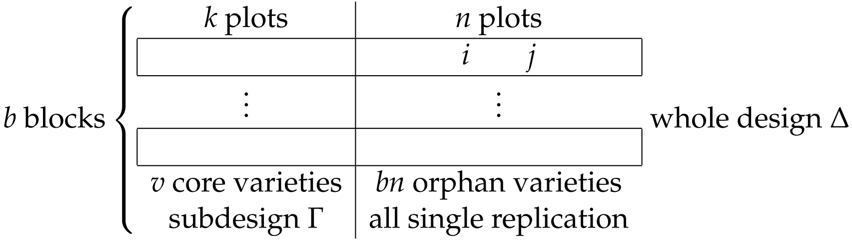
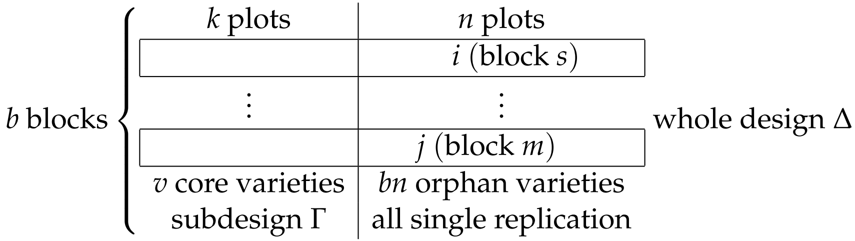


$$\mathrm{Var}_\Delta(\hat{\tau}_i - \hat{\tau}_j) = 2\sigma^2.$$

Pairwise variance: two orphans in different blocks

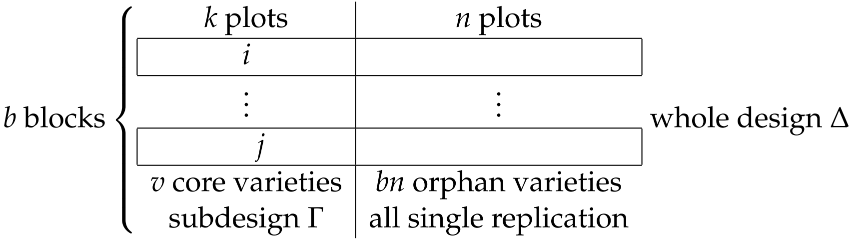


Pairwise variance: two orphans in different blocks

	k plots	n plots	
b blocks		i (block s)	
	$\vdots$	$\vdots$	whole design Δ
		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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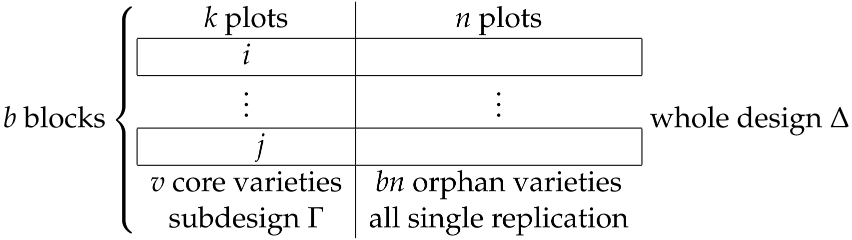
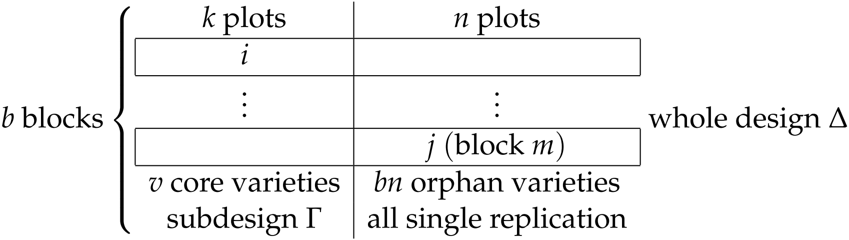


$$\mathrm{Var}_{\Delta}(\hat{\tau}_i - \hat{\tau}_j) = \mathrm{Var}_{\Gamma}(\hat{\tau}_i - \hat{\tau}_j).$$

Pairwise variance: one core variety and one orphan



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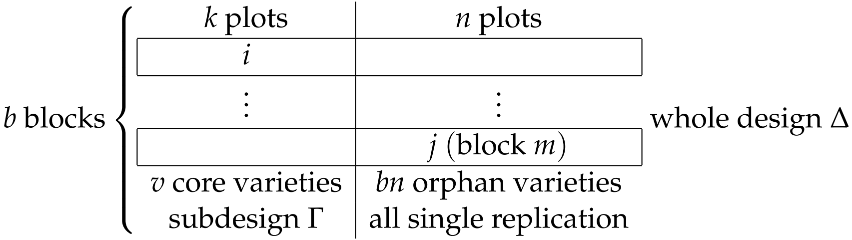

$$\mathrm{Var}_{\Delta}(\hat{\tau}_i - \hat{\tau}_j) = \sigma^2 + \mathrm{Var}_{\Gamma}(\hat{\tau}_i + \hat{\beta}_m).$$

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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(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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K_1	K_2	1	2	A_1	$\cdots$	A_n
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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

D-optimality

The block design is D-optimal if it minimizes
the volume of the ellipsoid of confidence for $(\tau_1, \ldots, \tau_{v+bn})$
in the hyperplane defined by

$$\sum_i \tau_i = 0.$$

Levi graph

The Levi graph of the block design has

- one vertex for each treatment

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Levi graph

The Levi graph of the block design has

- one vertex for each treatment
- one vertex for each block
- one edge for each plot,
  so that the edge corresponding to plot ω joins the vertices corresponding to treatment $g(\omega)$ and block $h(\omega)$.

Levi graph: example

1	2	3	4	A_1	$\cdots$	A_n
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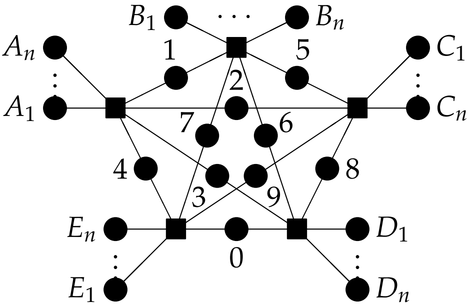

Spanning trees

A spanning tree for the Levi graph is a collection edges which provides a unique path between every pair of vertices.

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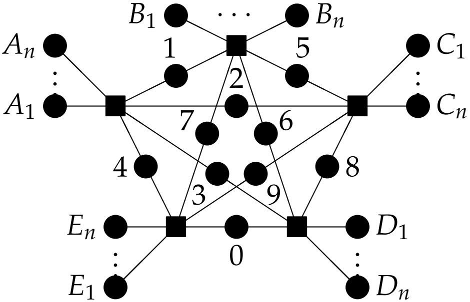

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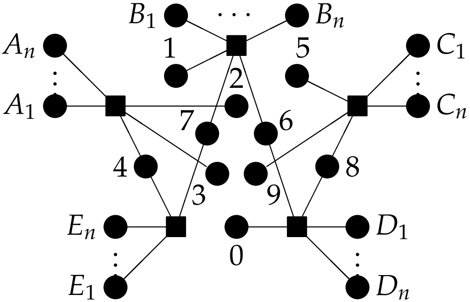

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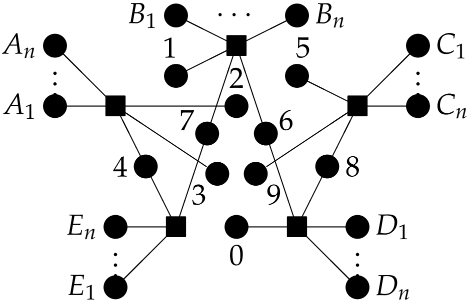

This Levi graph has 8000 spanning trees; the Levi graph for the chain block design has 5120 spanning trees.

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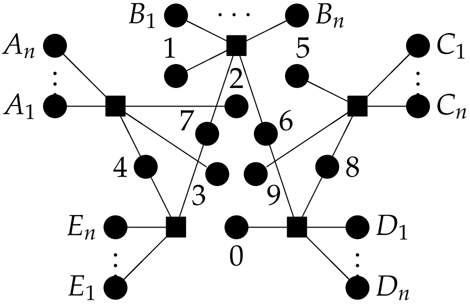

This Levi graph has 8000 spanning trees; the Levi graph for the chain block design has 5120 spanning trees.

The orphans make no difference to the number of spanning trees for the Levi graph.

Spanning trees and D-optimality

Theorem (Gaffke, 1981)

A block design is D-optimal if and only if its Levi graph maximizes the number of spanning trees.

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The whole design Δ is D-optimal
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Consequence

Even when n or b is large, D-optimal designs do not include uninteresting controls.