Optimal design of experiments with very low average replication

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Abstract

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The optimality criterion used is usually the A criterion: the average variance of the pairwise differences between the new varieties.

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
number of varieties $<$ number of plots $<<$ $2 \times$ 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

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

Simplest model

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

where

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

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

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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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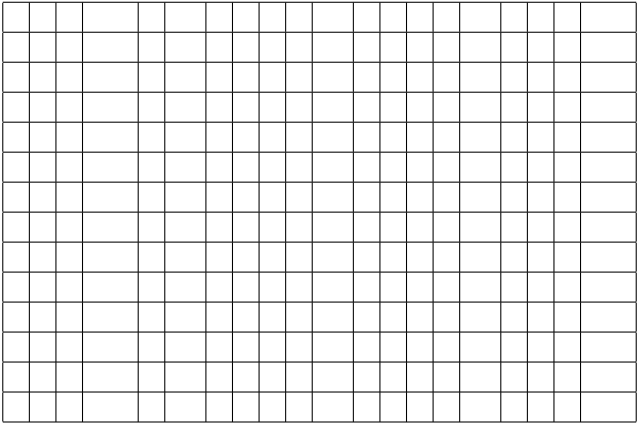

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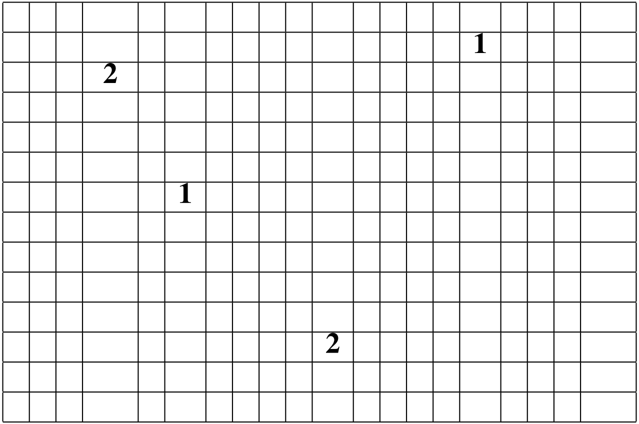

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															1				
			2																
																			57
					1														
			58																
									2										

A breeder says . . .

Unfair!

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

Fixed spatial trend

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

where

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

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Caliński, Mejza, ...:
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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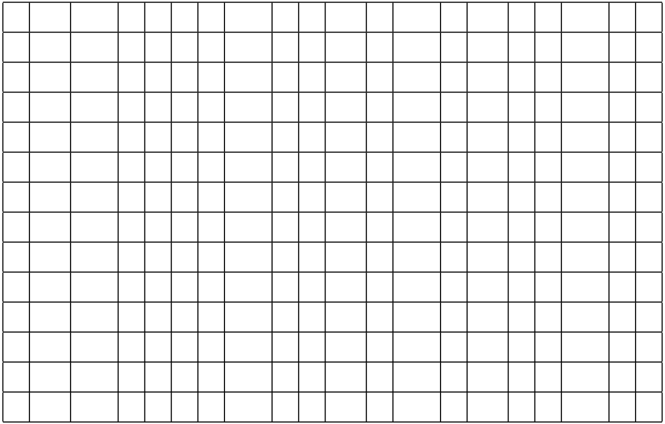

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		X					X					X					X		
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		X					**X**					**X**					**X**		
		X					**X**			**3**		**X**					**X**		
		X					**X**					**X**					**X**		
		X					**X**					**X**					**X**		
		X					**X**					**X**					**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**		
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(One block has all the stony plots; one block has all the plots near the rabbit warren, ...)

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

where

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

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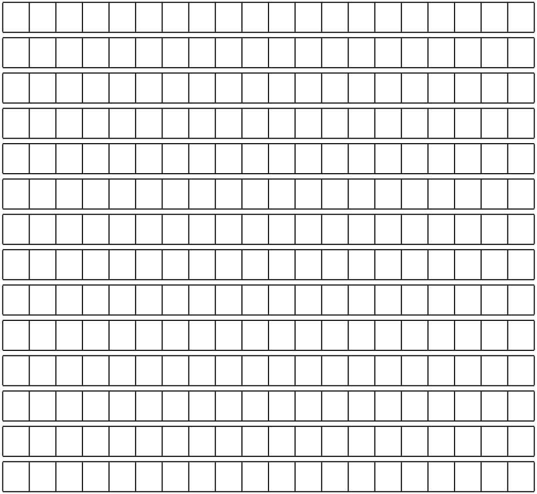
Blocks: example

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



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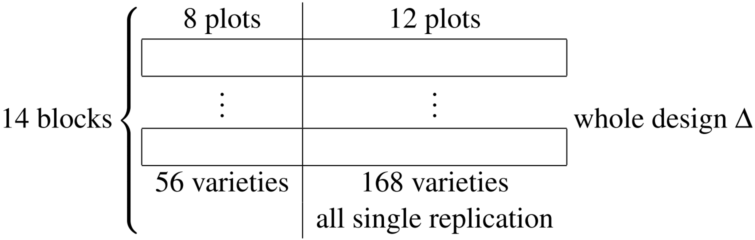
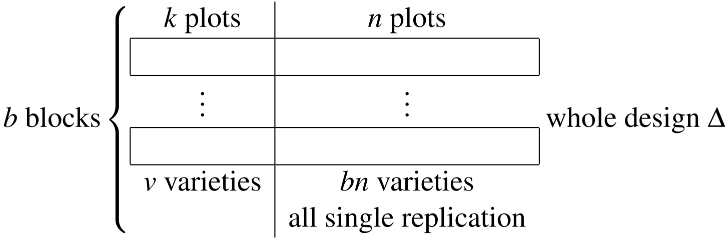


Subdesign Γ has 56 varieties
in 14 blocks of size 8.

A general block design with average replication less than 2



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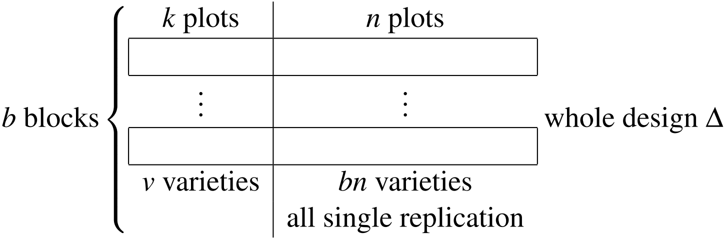

Whole design Δ has $v+bn$ varieties in b blocks of size $k+n$;

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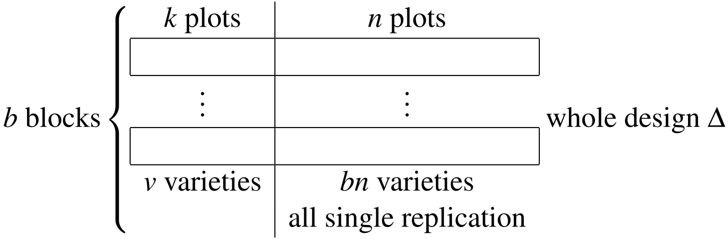

Whole design Δ has $v+bn$ varieties in b blocks of size $k+n$;
the subdesign Γ has v core varieties in b blocks of size k;

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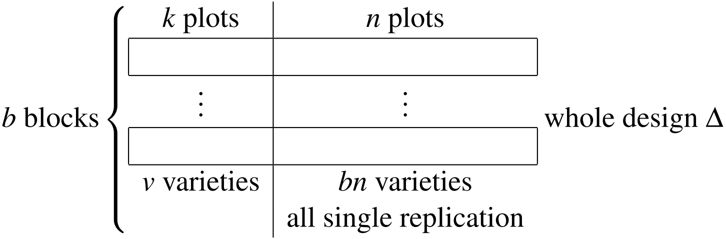
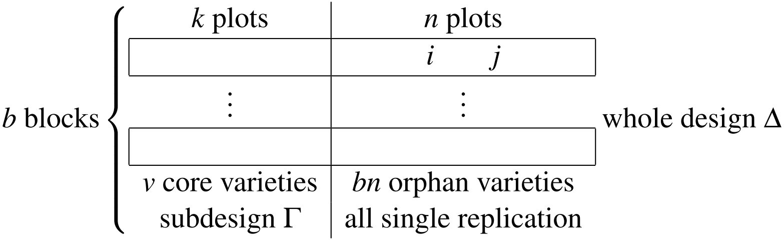


Whole design Δ has $v+bn$ varieties in b blocks of size $k+n$;
the subdesign Γ has v core varieties in b blocks of size k;
call the remaining varieties orphans.

Pairwise variance: two orphans in the same block



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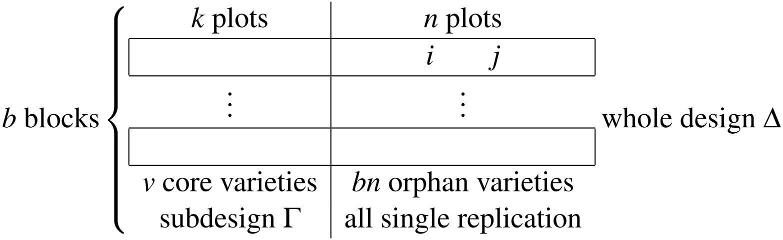
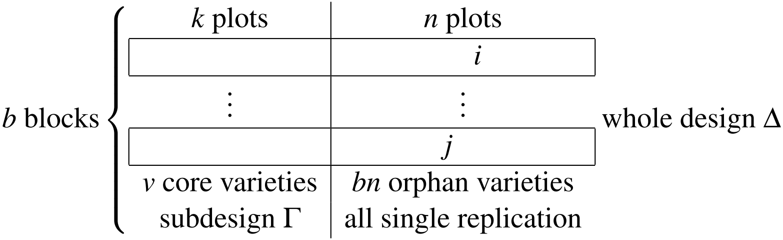


$$\mathrm{Var}_{\Delta}(\hat{\tau}_i - \hat{\tau}_j) = 2\sigma^2.$$

Pairwise variance: two orphans in different blocks



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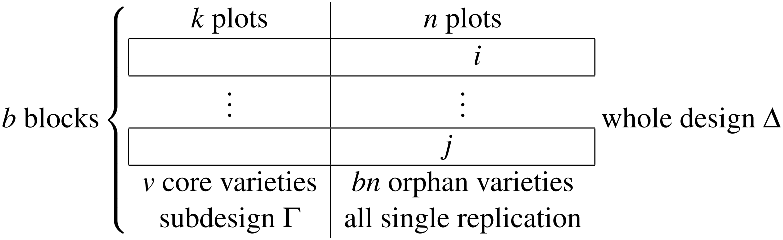
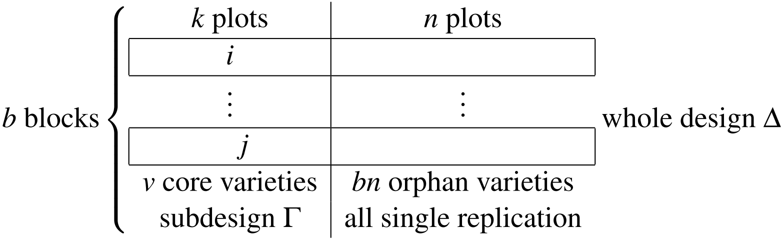


$$\mathrm{Var}_{\Delta}(\hat{\tau}_i - \hat{\tau}_j) = 2\sigma^2 + \mathrm{Var}_{\Gamma}(\hat{\beta}_i - \hat{\beta}_j).$$

Pairwise variance: two core varieties



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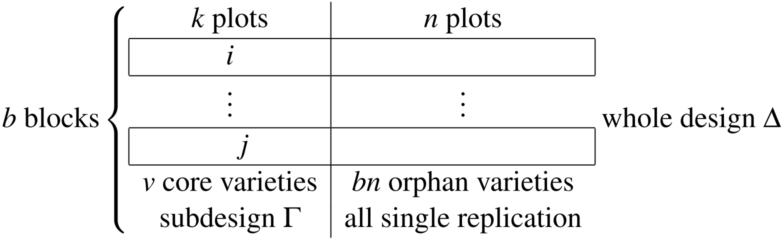

$$\mathrm{Var}_\Delta(\hat{\tau}_i - \hat{\tau}_j) = \mathrm{Var}_\Gamma(\hat{\tau}_i - \hat{\tau}_j).$$

Pairwise variance: one core variety and one orphan

b blocks (whole design Δ)

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

whole design Δ

Pairwise variance: one core variety and one orphan

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		j (block m)	
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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 increasing functions of V_1.)

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(If Γ is equi-replicate then V_2 and V_3 are 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" — chain block design

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

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

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

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

subdesign is dual of BIBD, best subdesign for $k = 4$

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

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

subdesign is dual of BIBD,
best subdesign for $k=4$

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

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

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

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

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4	5	1	9	D_1	$\cdots$	D_n
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