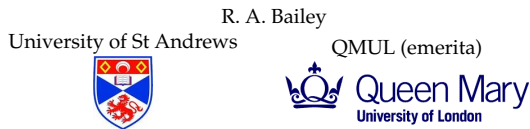


Designs for variety trials with very low replication



TU Dortmund, June 2015

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Abstract

In the early stages of testing new varieties, it is common that there are only small quantities of seed of many new varieties.

In the UK (and some other countries with centuries of agriculture on the same land) variation within a field can be well represented by a division into blocks.

Even when that is not the case, subsequent phases (such as testing for milling quality, or evaluation in a laboratory) have natural blocks, such as days or runs of a machine.

I will discuss how to arrange the varieties in a block design when the average replication is less than two.

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Variety Testing

In breeding trials of new varieties, typically there is very little seed of each of the new varieties.

Traditionally, an experiment has one plot for each new variety and several plots for a well-established "control":

for example,

New	Control	Total
30	1	31
1	8	38

In the last 12 years, Cullis and colleagues in Australia (and independently Bueno and Gilmour) have suggested replacing many occurrences of the the control by double replicates of a small number of new varieties:

for example,

New	New	Control	Total
24	6	1	31
1	2	2	38

This is an improvement if there are no blocks.

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How do we allow for variation between the plots?

"... on any given field agricultural operations, at least for centuries, have followed one of two directions, which are usually those of the rows and columns; consequently streaks of fertility, weed infestation, etc., do, in fact, occur predominantly in those two directions."

R. A. Fisher,
 letter to H. Jeffreys,
 30 May 1938
 (selected correspondence edited by J. H. Bennett)

(This assumption is dubious for field trials in Australia.)

If field operations have been primarily in one direction for a long time, then it is reasonable to divide the fields into blocks whose length runs along that direction.

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Blocking in the second phase: an example

The milling phase of a wheat variety trial has 224 varieties to be compared. Only 10 can be milled in any one day. The trial can take place over 28 days, so there are 28 blocks of size 10.

There are only $280 - 224 = 56$ experimental units "spare" for replication. How should these be allocated?

28 blocks

2 units	8 units
⋮	⋮
2 controls in every block	222 varieties 220 single replication

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Two possible designs for 224 varieties in 28 blocks of 10

28 blocks

2 units	8 units
⋮	⋮
2 controls in every block	222 varieties 220 single replication

28 blocks

4 units	6 units
⋮	⋮
56 varieties all replicated twice	168 varieties all single replication

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The problem

We are given b blocks of size k . We are given v varieties.
Assume that

$$\text{average replication} = \bar{r} = \frac{bk}{v} \leq 2.$$

How should we allocate varieties to blocks?

What makes a block design good?

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Linear model, estimation and variance

We measure the response Y on each unit in each block.

If that unit has variety i and block D , then we assume that

$$Y = \tau_i + \beta_D + \text{random noise},$$

where the random noise is independently normally distributed with zero mean and constant variance σ^2 .

We want to estimate all the simple differences $\tau_i - \tau_j$.

Put

$$V_{ij} \sigma^2 = \text{variance of the best linear unbiased estimator for } \tau_i - \tau_j.$$

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

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Optimality

Apart from the constant multiple σ^2 ,

$$V_{ij} = \text{variance of the BLUE for } \tau_i - \tau_j.$$

Put

$$V_T = \sum_{i=1}^{v-1} \sum_{j=i+1}^v V_{ij} = \text{sum of variances of variety differences.}$$

Definition

For given values of b (the number of blocks), k (the size of the blocks) and v (the number of varieties), a block design is **A-optimal** if it minimizes V_T .

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An example with $5n + 10$ varieties in 5 blocks of size $4 + n$

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

How do we calculate pairwise variances in a generic design?

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Levi graph

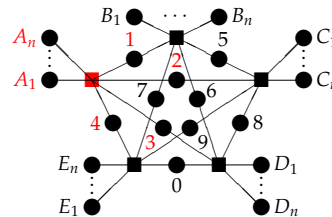
The **Levi graph** of the block design has

- ▶ one vertex for each variety
- ▶ one vertex for each block
- ▶ one edge for each plot (a.k.a. experimental unit), so that the edge for plot ω joins the vertex for the variety on ω to the vertex for the block containing ω .

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Levi graph: example

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



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Electrical networks

We can consider the Levi 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 whichever 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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Electrical networks: variance

Reminder: V_{ij} = variance of BLUE of $\tau_i - \tau_j$ for varieties i and j .

Theorem

If R_{ij} is the effective resistance between variety vertices i and j in the Levi graph then

$$R_{ij} = V_{ij}.$$

Put: V_{CD} = variance of BLUE of $\beta_C - \beta_D$ for blocks C and D ,
 V_{iC} = variance of BLUE of $\tau_i + \beta_C$ for variety i and block C .

Theorem

If R_{CD} and R_{iC} are the effective resistances between vertices C and D , and between i and C respectively, in the Levi graph then

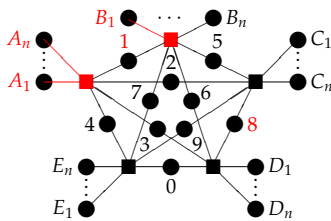
$$R_{CD} = V_{CD} \quad \text{and} \quad R_{iC} = V_{iC}.$$

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

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Pairwise resistance

(remove A_1, \dots, E_n to get core subdesign Γ)



$$\begin{aligned} \text{Resistance}(A_1, A_2) &= 2 \\ \text{Resistance}(A_1, B_1) &= 2 + \text{Resistance}(\text{block } A, \text{block } B) \text{ in } \Gamma \\ \text{Resistance}(A_1, 8) &= 1 + \text{Resistance}(\text{block } A, 8) \text{ in } \Gamma \\ \text{Resistance}(1, 8) &= \text{Resistance}(1, 8) \text{ in } \Gamma \end{aligned}$$

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Silly names just for this talk

Definition

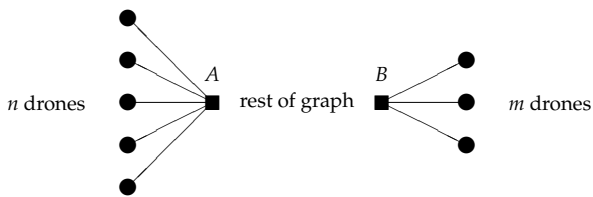
Call a variety a

- a **drone** if it has replication 1;
- a **queen-bee** if it occurs in every block;
- a **worker** otherwise.

Is it better to put all the drones into one block (or a few blocks), or are they better distributed equally among all the blocks?

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How should we distribute the drones?

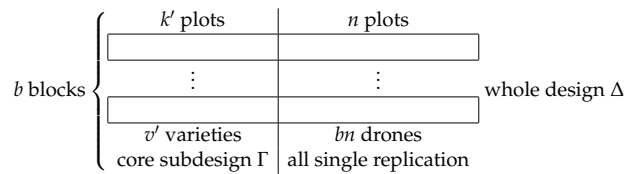


If we move all the drones in block B into block A then we reduce nm variances from $2 + R_{AB}$ to 2.

Then we have to remove m non-drones from block A , and this increases the resistance between A and the rest of the graph. This increases the variances between these $n + m$ drones and the remaining $v - n - m$ varieties. This more than compensates for the original reduction in variance.

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From now on, distribute drones as equally as possible



Whole design Δ has v treatments in b blocks of size $k = k' + n$; the **core subdesign** Γ has v' **core** varieties in b blocks of size k' , where $v' = v - bn$.
(The core varieties may include up to $b - 1$ extra drones.)

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Sum of the pairwise variances

Theorem (cf. Herzberg and Jarrett, 2007)

If there are n drones in each block of Δ , and the core subdesign Γ has v' varieties in b blocks of size k' then the sum of the variances of variety differences in Δ

$$= V_T(\Delta) = bn(bn + v' - 1) + V_T + nV_{BT} + n^2V_B,$$

where

- V_T = the sum of the variances of variety differences in Γ
- V_B = the sum of the variances of block differences in Γ
- V_{BT} = the sum of the variances of sums of one treatment and one block in Γ .

Sum of variances in whole design if Γ is equi-replicate

$$V_T(\Delta) = bn(bn + v' - 1) + V_T + nV_{BT} + n^2V_B$$

- V_T = the sum of the variances of variety differences in Γ
- V_B = the sum of the variances of block differences in Γ
- V_{BT} = the sum of the variances of sums of one treatment and one block in Γ .

If Γ is equi-replicate with replication r' then

$$\frac{k'}{b}V_B - b = \frac{r'}{v'}V_T - v';$$

$$V_{BT} = \frac{2b}{v'}V_T + \frac{v'}{k'}(b - v' - 1),$$

and so V_B and V_{BT} are both increasing functions of V_T .

Consequence

For a given choice of k' , use the core subdesign Γ which minimizes V_T .

Sum of variances in whole design if there are many drones

$$V_T(\Delta) = bn(bn + v' - 1) + V_T + nV_{BT} + n^2V_B$$

- V_T = the sum of the variances of variety differences in Γ
- V_B = the sum of the variances of block differences in Γ
- V_{BT} = the sum of the variances of sums of one treatment and one block in Γ .

Consequence

If n is large, we need to focus on reducing V_B , so it may be best to increase the number of drones and decrease k' (the size of blocks in the core subdesign 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	3	$n + 1$ drones
1	2	5	6	n drones	1	2	4	$n + 1$ drones
3	6	7	8	n drones	1	3	4	$n + 1$ drones
4	5	7	8	n drones	2	3	4	$n + 1$ drones

A definite result

Theorem (Duals of BIBDs cannot be beaten)

Suppose that we are given b blocks of size k , and v varieties. For $i = 1, 2$, let design Δ_i have core subdesign Γ_i with block size k_i . If Γ_1 is the dual of a balanced incomplete block design and $k_1 > k_2$ then Δ_2 is worse than Δ_1 on the A criterion, no matter how big v is.

Design	Δ_1	Δ_2
Core subdesign	Γ_1	Γ_2
block size in subdesign	k_1	k_2
property of core subdesign	dual of BIBD	arbitrary

$>$

then Δ_1 is A-better than Δ_2 .

An example of the good result

If there are $7(3 + n)$ varieties in 7 blocks of size $6 + n$, the design on the left is A-better than the design on the right, for all values of n .

1	2	3	4	5	6	n drones	1	4	6	7	$n + 2$ drones
1	7	8	9	10	11	n drones	1	2	5	7	$n + 2$ drones
2	7	12	13	14	15	n drones	1	2	3	6	$n + 2$ drones
3	8	12	16	17	18	n drones	2	3	4	7	$n + 2$ drones
4	9	13	16	19	20	n drones	1	3	4	5	$n + 2$ drones
5	10	14	17	19	21	n drones	2	4	5	6	$n + 2$ drones
6	11	15	18	20	21	n drones	3	5	6	7	$n + 2$ drones

Another example of the good result

If there are $4n + 6$ varieties in 4 blocks of size $3 + n$, the design on the left is A-better than the design on the right, for all values of n .

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

1	2	$n + 1$ drones
1	2	$n + 1$ drones
1	2	$n + 1$ drones
1	2	$n + 1$ drones

Strategy

Given b, v and k , how do we find an A-optimal design for v varieties in b blocks of size k when

$$\frac{bk}{2} \leq v \leq b(k-1) + 1?$$

Average replication ≤ 2 Maximum v for estimability

- Case 1. $b = 2$ or $b = 3$ (very small b).
- Case 2. $v = b(k-1) + 1$ or $v = b(k-1)$ (very large v).
- Case 3. $k_0 \geq b - 1$.
- Case 4. $2 < k_0 < b - 1$ (small k_0 but not Case 2).

$$k_0 = k - \left\lfloor \frac{2v - bk}{b} \right\rfloor = \text{biggest space per block for non-drones.}$$

Case 1. Only 2 blocks, of size k

Morgan and Jin (2007) showed that the A-optimal designs are those with $2n$ drones and q queen bees, where $n = n_0 = v - k$ and $q = k' = k_0 = k - n_0 = 2k - v$.

1	2	3	4	...	q	A_1	A_2	A_3	...	A_n
1	2	3	4	...	q	B_1	B_2	B_3	...	B_n

queens drones

Case 1 continued. 3 blocks of size k

Using the result about drone-distribution and the nice theorem about duals of BIBDs, RAB has shown that the A-optimal designs are as follows when v is divisible by 3 (and presumably small changes deal with the other cases). There are $3w$ workers and $3n$ drones, where $3w = 3k - v$ and $n = n_0 = k - 2w$ and $k' = k_0 = 2w$.

1	2	4	5	...	$3w - 2$	$3w - 1$	A_1	A_2	A_3	...	A_n
1	3	4	6	...	$3w - 2$	$3w$	B_1	B_2	B_3	...	B_n
2	3	5	6	...	$3w - 1$	$3w$	C_1	C_2	C_3	...	C_n

w copies of design using all pairs from 3 drones

Case 2. $v = b(k-1) + 1$

This is the maximum number of varieties that can be tested in b blocks of size k with all comparisons estimable.

Mandal, Shah and Sinha (1991), for $k = 2$, Dean and co-authors, and Bailey and Cameron (2013), for general block size, showed that, no matter how many blocks there are, the A-optimal design has the following form.

1	A_1	A_2	A_3	...	A_{k-1}
1	B_1	B_2	B_3	...	B_{k-1}
1	C_1	C_2	C_3	...	C_{k-1}
1	D_1	D_2	D_3	...	D_{k-1}
1	E_1	E_2	E_3	...	E_{k-1}

1 queen $v - 1$ drones

Case 2 continued. $v = b(k-1)$

The A-optimal designs were found for all cases by Krafft and Schaefer (1997).

small k and b increase k if $b \geq 5$ then increase b

1	2	A_1
2	3	B_1
3	4	C_1
4	5	D_1
5	6	E_1
6	1	F_1

chain

1	2	A_1	A_2
2	3	B_1	B_2
3	1	C_1	C_2
1	D_1	D_2	D_3
1	E_1	E_2	E_3
1	F_1	F_2	F_3

smaller chain

1	2	A_1	A_2
1	2	B_1	B_2
1	C_1	C_2	C_3
1	D_1	D_2	D_3
1	E_1	E_2	E_3
1	F_1	F_2	F_3
1	G_1	G_2	G_3

1 queen

Youden and Connor (1953) had recommended chain designs.

Case 3. A bad example: $b = 4$ and $k_0 = 4$

$v = 4n + 8$ and $k = 4 + n$

My strategy gives

1	2	3	7	A_1	...	A_n
1	4	5	7	B_1	...	B_n
2	4	6	8	C_1	...	C_n
3	5	6	8	D_1	...	D_n
			Γ_0	drones		

which is worse than

1	2	3	A_1	...	A_{n+1}
1	2	4	B_1	...	B_{n+1}
1	3	4	C_1	...	C_{n+1}
2	3	4	D_1	...	D_{n+1}
			$k' = 3$	drones	
			rep 3		

when $n \geq 50$.

Case 4. $2 < k_0 < b - 1$

For various values of $k_i \leq k_0$, find the best core subdesign Γ_i for v'_i varieties in b blocks of size k_i . (For equi-replicate core subdesigns, it is often easier to find the best dual design, which is obtained by interchanging the roles of blocks and varieties.)

- $V_T(\Gamma_i)$ = the sum of the variances of variety differences in Γ_i
- $V_B(\Gamma_i)$ = the sum of the variances of block differences in Γ_i
- $V_{BT}(\Gamma_i)$ = the sum of the variances of sums of one treatment and one block in Γ_i .

If there are n_i drones in each block then, in the whole design Δ ,

$V_T(\Delta) = bn_i(bn_i + v'_i - 1) + V_T(\Gamma_i) + n_i V_{BT}(\Gamma_i) + n_i^2 V_B(\Gamma_i)$.

Use this formula to find the core subdesign which gives the smallest $V_T(\Delta)$.

As the number of varieties increases, it becomes more important to choose Γ_i with a small value of $V_B(\Gamma_i)$.

Case 4 continued. $k_0 = 4 < b - 1$, $V_B(\Gamma_i) \div b(b - 1)/2$

Best design for b blocks known to RAB

k_i	Γ_1 2 2 queens, both boring	Γ_2 3 2 queens, 2 workers (rep 2)	Γ_3 3 b workers rep 3	Γ_4 4 $2b$ workers rep 2
$b = 6$	1	1 ⁻	0.85	0.87
$b = 7$	1	1 ⁻	0.86	0.92
$b = 8$	1	1 ⁻	0.89	0.93
$b = 9$	1	1 ⁻	0.92	
$b = 10$	1	1 ⁻		
$b = 11$	1	1 ⁻		
$b = 12$	1	1 ⁻	0.98	
$b = 13$	1	1 ⁻	1	1.07
$b = 14$	1	1 ⁻		
$b = 15$	1	1 ⁻	1.01	1.08

As v increases, Γ_3 becomes better than Γ_4 .
If $b \geq 14$, then, as v increases, Γ_1 and Γ_2 become better than Γ_3 .

Case 4 continued. $2 < k_0 < b - 1$ when $b = 8$: $k_0 = 6$

$k = k_0 = 6$, and 24 varieties, all workers, all replicated twice.

1	2	3	4	5	6
7	8	9	10	11	12
1	7	13	14	15	16
2	8	17	18	19	20
3	9	13	17	21	22
4	10	14	18	23	24
5	11	15	19	21	23
6	12	16	20	22	24

(One worker for each pair of blocks except for $\{A, B\}$, $\{C, D\}$, $\{E, F\}$ and $\{G, H\}$.)

Case 4 continued. $k = 5$ and $k = 6$ when $b = 8$: $k_0 = 5$

$k = 5$
20 varieties:
20 workers, no drones

1	2	3	4	5
6	7	8	9	10
1	11	12	13	14
2	6	15	16	17
3	7	11	18	19
4	8	12	15	20
5	9	13	16	18
10	14	17	19	20

$k = 6$
28 varieties:
20 workers, 8 drones

1	2	3	4	5	A_1
6	7	8	9	10	B_1
1	11	12	13	14	C_1
2	6	15	16	17	D_1
3	7	11	18	19	E_1
4	8	12	15	20	F_1
5	9	13	16	18	G_1
10	14	17	19	20	H_1

Case 4 continued. $k = 5$ and $k = 6$ when $b = 8$: $k_0 = 4$

$k = 5$
24 varieties:
16 workers, 8 drones

1	2	3	4	A_1
5	6	7	8	B_1
9	10	11	12	C_1
13	14	15	16	D_1
1	5	9	13	E_1
2	6	10	14	F_1
3	7	11	15	G_1
4	8	12	16	H_1
				$k' = 4$
				rep = 2

$k = 6$
32 varieties:
8 workers, 24 drones

1	2	4	A_1	A_2	A_3
2	3	5	B_1	B_2	B_3
3	4	6	C_1	C_2	C_3
4	5	7	D_1	D_2	D_3
5	6	8	E_1	E_2	E_3
6	7	1	F_1	F_2	F_3
7	8	2	G_1	G_2	G_3
8	1	3	H_1	H_2	H_3
				$k' = 3$	
				rep 3	

Case 4 continued. $k = 5$ and $k = 6$ when $b = 8$: $k_0 = 3$

$k = 5$
28 varieties:
12 workers, 16 drones

1	2	3	A_1	A_2
1	4	5	B_1	B_2
4	6	7	C_1	C_2
6	8	9	D_1	D_2
2	8	10	E_1	E_2
5	10	11	F_1	F_2
7	11	12	G_1	G_2
3	9	12	H_1	H_2

$k = 6$
36 varieties:
12 workers, 24 drones

1	2	3	A_1	A_2	A_3
1	4	5	B_1	B_2	B_3
4	6	7	C_1	C_2	C_3
6	8	9	D_1	D_2	D_3
2	8	10	E_1	E_2	E_3
5	10	11	F_1	F_2	F_3
7	11	12	G_1	G_2	G_3
3	9	12	H_1	H_2	H_3

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Health Warning

The overall message is that there can be phase changes as the spare capacity for replication ($bk - v$) decreases. Therefore it is necessary to compare core subdesigns Γ_i with different block size k_i .

Although this overall message is correct, no one has checked the arithmetic in the examples presented, so individual cases may be wrong.

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Warning for specialists in optimality

The results given are for A-optimality.

A design is MV-optimal if it minimizes the value of the maximal V_{ij} .

If $2v - bk \leq k - 1$ then it is possible to put all the drones in a single block, and the MV-optimal design may have this form.

A design is D-optimal if it minimizes the volume of the confidence ellipsoid for the vector of fitted values (τ_1, τ_2, \dots) under the assumption of independent identically distributed normal errors.

The D-optimal designs have core subdesigns with the largest possible value of k' (and so the smallest possible number of drones), no matter how large the number of varieties.

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