Block designs with very low replication, and other challenges in design of experiments

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Variety Testing

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Traditionally, an experiment has one plot for each new variety and several plots for a well-established “control”: for example, 30 new varieties on one plot each and one control on 8 plots.

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have suggested replacing many occurrences of the the control by double replicates of a small number of new varieties: for example, 24 new varieties with one plot each, 6 new varieties with two plots each, and the control on two further plots.

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This is an improvement if there are no blocks.

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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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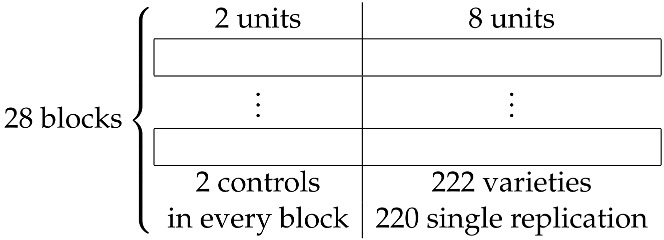

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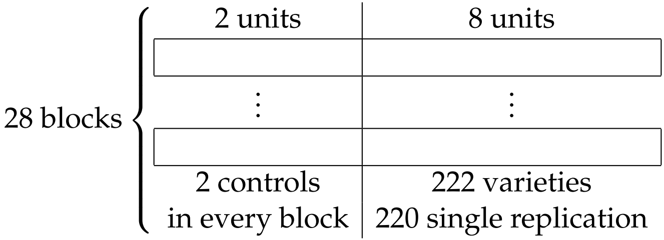
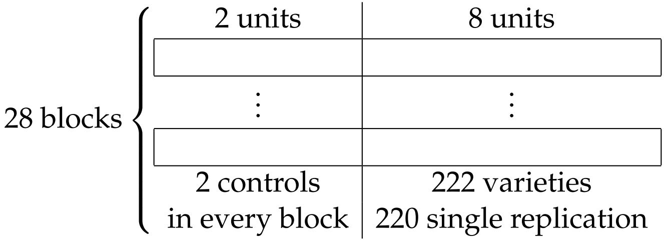


One extreme: 2 "controls" (among the test varieties) in every block.
Even more extreme: 2 uninteresting controls in each block.

Two possible designs for 224 varieties in 28 blocks of 10



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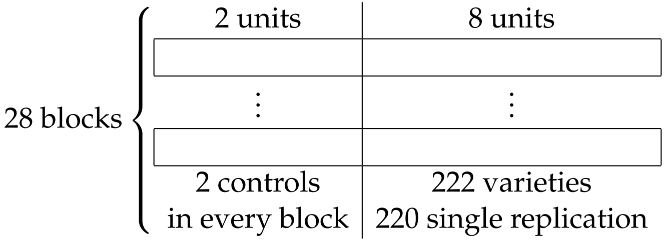

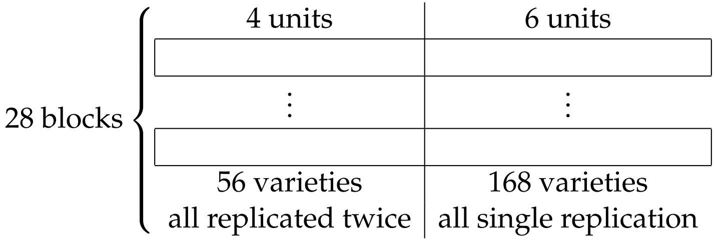

The problem

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?

A-optimal designs

We measure the response Y on the plot with variety i in block D, and assume that

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

where the random noise is $N(0, \sigma^2)$, independently for each plot.

Put

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

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

A block design is A-optimal if it minimizes V_T.

Silly names just for this talk

Definition

Call a variety a

a drone if it has replication 1;

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- a drone if it has replication 1;
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- 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?

How should we distribute the drones?

Block A	Block B
n drones	m drones

If we move all the drones in block B into block A
then we reduce nm variances from $2 + V_{AB}$ to 2,
where V_{AB} is the variance of the estimator of the difference between the block effects of A and B in the design obtained by ignoring the drones.

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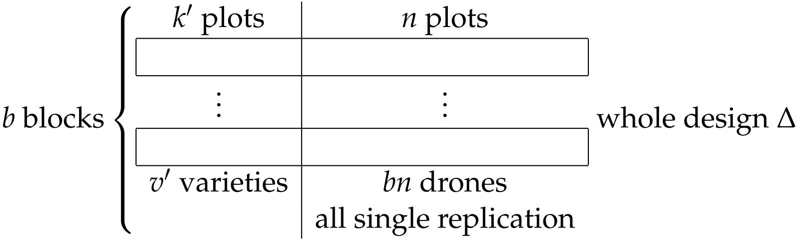
Then we have to remove m non-drones from block A,
and this increases the variances between these $n + m$ drones and the remaining $v - n - m$ varieties. This more than compensates for the original reduction in variance.

From now on, distribute drones as equally as possible



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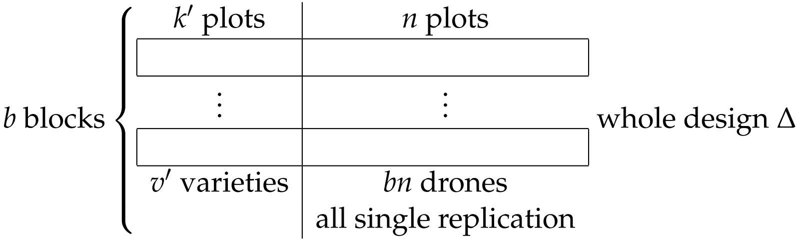

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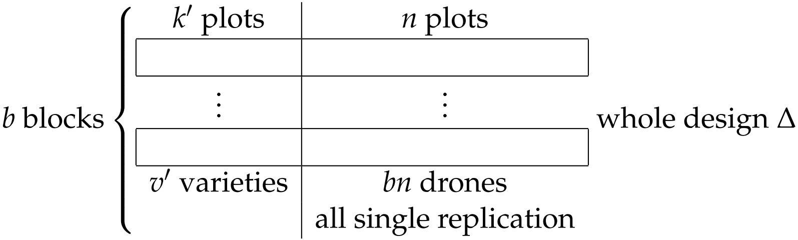

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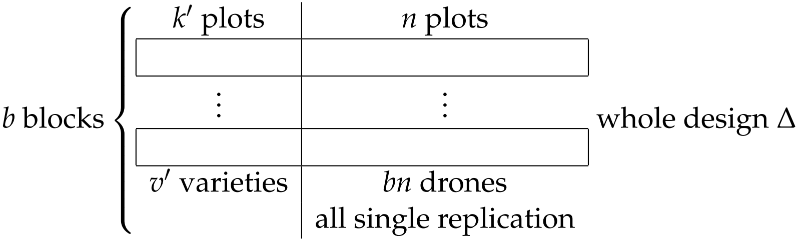

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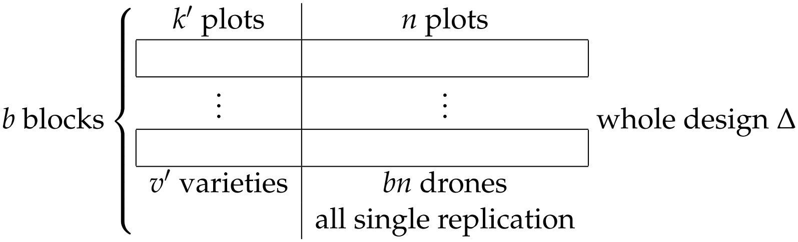

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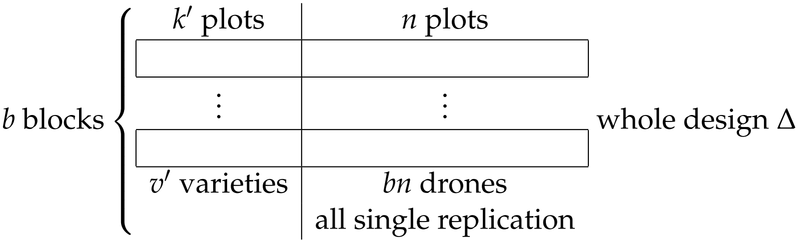

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Sum of the pairwise variances

Theorem (cf. Herzberg and Jarrett, 2007)

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

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

where

$$\begin{aligned} V_T(\Gamma) &= \text{the sum of the variances of variety differences in } \Gamma \\ V_B(\Gamma) &= \text{the sum of the variances of block differences in } \Gamma \\ V_{BT}(\Gamma) &= \text{the sum of the variances of sums of} \\ &\quad \text{one treatment and one block in } \Gamma. \end{aligned}$$

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If Γ is equi-replicate with replication r' then

$$\begin{aligned} \frac{k'}{b} V_B(\Gamma) - b &= \frac{r'}{v'} V_T(\Gamma) - v'; \\ V_{BT}(\Gamma) &= \frac{2b}{v'} V_T(\Gamma) + \frac{v'}{k'}(b - v' - 1), \end{aligned}$$

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Consequence

For a given choice of k', use the core design Γ which minimizes $V_T(\Gamma)$.

Sum of variances in whole design if there are many drones

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Consequence

If v is large then n is large, so we need to focus on reducing $V_B(\Gamma)$,
so it may be best to increase the number of drones
and decrease k' (the size of blocks in the core design 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	5	6	n drones
3	6	7	8	n drones
4	5	7	8	n drones

1	2	3	$n+1$ drones
1	2	4	$n+1$ drones
1	3	4	$n+1$ drones
2	3	4	$n+1$ drones

A definite result

Theorem

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.

An 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
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Strategy

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

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Case 3. $k_0 \geq b-1$.

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

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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	$\ldots$	q	A_1	A_2	A_3	$\ldots$	A_n
1	2	3	4	$\ldots$	q	B_1	B_2	B_3	$\ldots$	B_n
queens						drones				

Case 1 continued. 3 blocks of size k

Using the nice theorem, 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 $k=2$,
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	$\dots$	A_{k-1}
1	B_1	B_2	B_3	$\dots$	B_{k-1}
1	C_1	C_2	C_3	$\dots$	C_{k-1}
1	D_1	D_2	D_3	$\dots$	D_{k-1}
1	E_1	E_2	E_3	$\dots$	E_{k-1}
1 queen	$v-1$ drones				

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

The A-optimal designs were found for all cases
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small k and 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

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

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

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1	D_1	D_2	D_3
1	E_1	E_2	E_3
1	F_1	F_2	F_3

smaller chain

then increase b

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

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

1	2	A_1
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smaller chain

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Youden and Connor (1953) had recommended chain designs.

Case 3. $k \geq k_0 \geq b - 1$

For simplicity, assume that b divides $2v$, so that

$$n_0 = \frac{2v - bk}{b} = \text{minimum number of drones per block.}$$

Then

$$\frac{b(2k - b + 1)}{2} \geq v \geq \frac{bk}{2} \geq \frac{b(b-1)}{2}.$$

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Then

$$\frac{b(2k - b + 1)}{2} \geq v \geq \frac{bk}{2} \geq \frac{b(b-1)}{2}.$$

Let Γ_0 be the design for $b(b-1)/2$ varieties
replicated twice in b blocks of size $b - 1$
in such a way that
there is one variety in common to each pair of blocks.
This is A-optimal for these numbers.

Case 3 continued. $k \geq k_0 \geq b - 1$

If $k_0 = s(b-1)$ then take Γ to be s copies of Γ_0.
This is always A-optimal.

Case 3 continued. $k \geq k_0 \geq b - 1$

If $k_0 > b - 1$ but k_0 is not a multiple of $b - 1$,
then the following strategy seems likely to be good
(but it is not A-optimal when $b = k_0 = 4$ and v is very large).

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(but it is not A-optimal when $b = k_0 = 4$ and v is very large).
$n_0 =$ minimal number of drones per block.

Construction Method

1. *put n_0 drones in each block;*

Case 3 continued. $k \geq k_0 \geq b - 1$

If $k_0 > b - 1$ but k_0 is not a multiple of $b - 1$,
then the following strategy seems likely to be good
(but it is not A-optimal when $b = k_0 = 4$ and v is very large).
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Construction Method

1. *put n_0 drones in each block;*
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Construction Method

1. *put n_0 drones in each block;*
2. *put in one copy of Γ_0;*
3. *put in as many further copies of Γ_0 as possible;*

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Construction Method

1. *put n_0 drones in each block;*
2. *put in one copy of Γ_0;*
3. *put in as many further copies of Γ_0 as possible;*
4. *in any remaining space,*
   use a good design for workers with replication 2
   (so long as there is at least one copy of Γ_0,
   it probably doesn't make much difference which one is used).

Case 3. Example: $b = 8$ and $k = 15$ (so $60 \leq v \leq 92$)

60 varieties: all workers ($n_0 = 0$)

1	2	3	4	5	6	7	29	30	31	32	33	34	35	57
1	8	9	10	11	12	13	29	36	37	38	39	40	41	57
2	8	14	15	16	17	18	30	36	42	43	44	45	46	58
3	9	14	19	20	21	22	31	37	42	47	48	49	50	58
4	10	15	19	23	24	25	32	38	43	47	51	52	53	59
5	11	16	20	23	26	27	33	39	44	48	51	54	55	59
6	12	17	21	24	26	28	34	40	45	49	52	54	56	60
7	13	18	22	25	27	28	35	41	46	50	53	55	56	60
one copy of Γ_0							another copy of Γ_0							

Case 3. Example: $b = 8$ and $k = 15$ (so $60 \leq v \leq 92$)

76 varieties: 44 workers, 32 drones ($n_0 = 4$)

1	2	3	4	5	6	7	29	30	31	32	A_1	A_2	A_3	A_4
1	8	9	10	11	12	13	33	34	35	36	B_1	B_2	B_3	B_4
2	8	14	15	16	17	18	37	38	39	40	C_1	C_2	C_3	C_4
3	9	14	19	20	21	22	41	42	43	44	D_1	D_2	D_3	D_4
4	10	15	19	23	24	25	29	33	37	41	E_1	E_2	E_3	E_4
5	11	16	20	23	26	27	30	34	38	42	F_1	F_2	F_3	F_4
6	12	17	21	24	26	28	31	35	39	43	G_1	G_2	G_3	G_4
7	13	18	22	25	27	28	32	36	40	44	H_1	H_2	H_3	H_4
Γ_0							16 workers replication 2				drones			

Case 3. Example: $b = 8$ and $k = 15$ (so $60 \leq v \leq 92$)

92 varieties: 28 workers, 64 drones ($n_0 = 8$)

1	2	3	4	5	6	7	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8
1	8	9	10	11	12	13	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8
2	8	14	15	16	17	18	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
3	9	14	19	20	21	22	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8
4	10	15	19	23	24	25	E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8
5	11	16	20	23	26	27	F_1	F_2	F_3	F_4	F_5	F_6	F_7	F_8
6	12	17	21	24	26	28	G_1	G_2	G_3	G_4	G_5	G_6	G_7	G_8
7	13	18	22	25	27	28	H_1	H_2	H_3	H_4	H_5	H_6	H_7	H_8

Γ_0 | drones

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For various values of $k_i \leq k_0$,
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\begin{aligned}
V_T(\Gamma_i) &= \text{the sum of the variances of variety differences in } \Gamma_i \\
V_B(\Gamma_i) &= \text{the sum of the variances of block differences in } \Gamma_i \\
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&\quad\ \text{one treatment and one block in } \Gamma_i.
\end{aligned}
$$

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

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

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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

	Γ_1	Γ_2	Γ_3	Γ_4
k_i	2	3	3	4
	2 queens, both boring	2 queens, 2 workers (rep 2)	b workers rep 3	$2b$ 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

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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

Health Warnings

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.

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This is work is progress, not a finished project.

The cornerstones of experimental design

- Replication.
- Blocking.
- Randomization.

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What is old?
What is new?

Replication: the old. I

In 2012 the UK's Food and Environment Research Agency conducted an experiment to find out "the effects of neonicotinoid seed treatments on bumble bee colonies under field conditions" (from a DEFRA report available on the web, Crown copyright 2013).

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Site	Treatment of oilseed rape seeds
Site A, near Lincoln	no treatment
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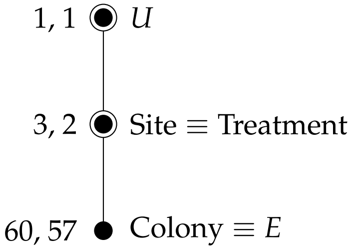
Twenty colonies of bumble bees were placed at each site. Various outcomes were measured on each colony.

Replication: the old. II



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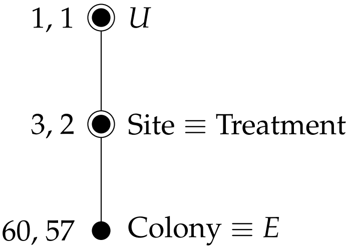

Skeleton analysis of variance

Stratum	Source	df
U	Mean	1
Sites	Treatments	2
Colonies		57

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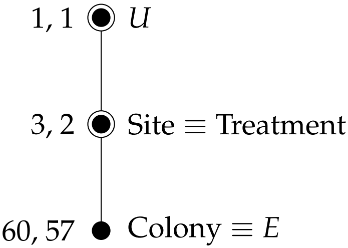

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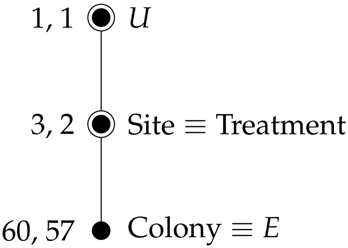

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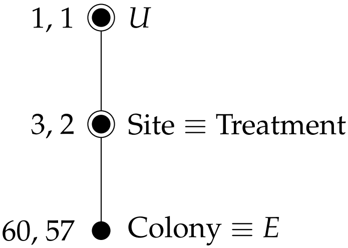

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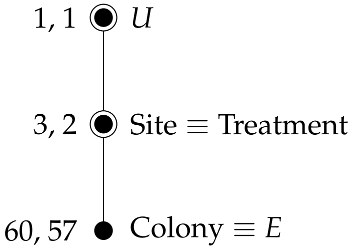

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The Hasse diagram can clearly show such false replication before the experiment is carried out.

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False replication is one of the oldest and most common mistakes in design of experiments.

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Why is it still happening in experiments undertaken or commissioned by publicly funded bodies?

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For example, Ching-Shui Cheng discussed supersaturated designs (for m 2-level factors in n experimental units, with $n < m$). One of the classical surrogates for model identifability is equal replication ("balance") of the levels of each factor. He showed that this is not a good guide when the models have high dimension.

Blocking: the old. I

The old paradigm is to group the experimental units into *blocks* of alike units,
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We know how to do this for several systems of blocks, under orthogonality.

Blocking: the old. II

In experiments in human-computer interaction, it is common to ask each participant to undertake a certain task under several different scenarios. With four scenarios, the experiment might use 20 participants once each on four days, and assign scenarios using Latin squares.

A	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*
B	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*
C	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*
D	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*	*D*	*A*	*B*	*C*

Blocking: the old. III

Skeleton analysis of variance

Stratum	Source	df
U	Mean	1
Days		3
Participants		19
Days#Participants	Scenarios	3
	residual	54

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This is wrong on two counts:

(i) We do not test for differences between days and between participants: we expect such differences and fit them in the model.

(ii) If we do not remove these differences, we decrease the power for detecting differences between scenarios.

Blocking: the new. I

As new technologies are used in experimentation
(for example, in genomics)
there may be systems of blocks which the experimenters do not recognise because they are not called ‘blocks’.
How do we ensure that known methods of construction, randomization and data analysis are not lost?

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How do we ensure that known methods of construction, randomization and data analysis are not lost?

In agricultural fields in some countries,
it is more realistic to model spatial variation by spatial correlation than by discrete blocks.
How should we construct and randomize such experiments, and analyse data from them?

Blocking: the new. II

In some recent experiments, the experimental units can be thought of as the nodes of a graph, with edges between some nodes. For example, Gerry Humphris of the University of St Andrews is experimenting with non-medical interventions such as sending a text message to known binge drinkers on Friday afternoons. One drinker (a node) may alter his behaviour and thus affect the behaviour of other people that he knows (the nodes joined to him in the graph).
How should we construct and randomize such experiments, and analyse data from them?

Randomization: the old. I

There is a large body of theory about how to randomize experiments in *simple orthogonal block structures* in such a way that estimators of treatment effects and of their variances are both unbiased over the randomization.

Randomization: the old. II

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- W. J. Youden: Randomization and experimentation. *Technometrics* **14**, (1972), 13–22.

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This has not stopped people from developing software for throwing away "undesirable" outcomes of randomization.

- D. T. Bowman: TFPlan: software for restricted randomization in field plot design. *Agronomy Journal* **92**, (2000), 1276–1278.
- A talk presented at the Tenth Working Seminar on Statistical Methods in Variety Testing at Będlewo, Poland, in July 2014.

Randomization: the new

For spatial correlation, and for designs on the nodes of graphs,

- how should we randomize?
- what criterion of validity should we use?