Conflicts between optimality criteria for block designs with low replication



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Ongoing joint work with Alia Sajjad and Peter Cameron

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I have *v* treatments that I want to compare. I have *b* blocks, with space for *k* treatments (not necessarily distinct) in each block. How should I choose a block design? Two designs with v = 5, b = 7, k = 3: which is better?



binary

non-binary

A design is binary is no treatment occurs more than once in any block.

1	1	2	3	4	5	6
2	4	5	6	10	11	12
3	7	8	9	13	14	15

1	1	1	1	1	1	1
2	4	6	8	10	12	14
3	5	7	9	11	13	15

replications differ by ≤ 1

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.

1	2	3	4	5	6	7	1	2	3	4	5	6	7
2	3	4	5	6	7	1	2	3	4	5	6	7	1
4	5	6	7	1	2	3	3	4	5	6	7	1	2

balanced (2-design)

non-balanced

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A binary design is balanced if every pair of distinct treaments occurs together in the same number of blocks.

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

1	1	2	3	4	5	6
2	4	5	6	10	11	12
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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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- \iff the graph *G* is connected
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Call the remaining eigenvalues nontrivial. They are all non-negative.

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.

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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

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

where $\theta_1, \ldots, \theta_{\nu-1}$ are the nontrivial eigenvalues of $L_{\mathbb{P}}$, where $\theta_1, \ldots, \theta_{\nu-1}$ are the nontrivial eigenvalues of $L_{\mathbb{P}}$.

Optimality

The design is called

• A-optimal if it minimizes the average of the variances V_{ij} ;

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- ► D-optimal if it minimizes the volume of the confidence ellipsoid for (τ₁,..., τ_v);

—equivalently, it maximizes the geometric mean of the non-trivial eigenvalues of the Laplacian matrix *L*;

E-optimal if minimizes the largest value of x^TL⁻x/x^Tx;
 —equivalently, it maximizes the minimum non-trivial eigenvalue θ₁ of the Laplacian matrix L:

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.

A spanning tree for the graph is a collection of edges of the graph which form a tree (graph with no cycles) and which include every vertex. A spanning tree for the graph is a collection of edges of the graph which form a tree (graph with no cycles) and which include every vertex.

Cheng (1981), after Gaffke (1978), after Kirchhoff (1847):

product of non-trivial eigenvalues of $L = v \times$ number of spanning trees

So a design is D-optimal iff its concurrence graph has the maximal number of spanning trees.

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So a design is D-optimal iff its concurrence graph has the maximal number of spanning trees.

This is easy to calculate by hand when the graph is sparse.

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.

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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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

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

If k = 2 then the design is the same as its concurrence graph, and connectivity requires $b \ge v - 1$.

If b = v - 1 then all connected designs are trees. The D-criterion does not differentiate them. The only A- or E-optimal designs are the stars.
If k = 2 and b = v then the design consists of a cycle with trees attached to some vertices.



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



The cycle is uniquely D-optimal when b = v.

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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.

D-optimal designs	cycle	always
A-optimal designs	cycle square with leaves attached triangle with leaves attached	$if v \le 8$ if $9 \le v \le 12$ if $12 \le v$
E-optimal designs	cycle triangle or digon with leaves	$if v \le 6 \\ if 6 \le v$

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For $v \ge 9$, the ranking on the D-criterion is essentially the opposite of the rankings on the A- and E-criteria and the A- and E-optimal designs are far from equi-replicate. The change is sudden, not gradual.

An old collaborator, 1980s

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That old collaborator, December 2008

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

The remaining arguments extend easily to general block size.

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

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.





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3⁷ spanning trees

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

 $\theta_1 \ge 1$

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

If 2b = v then *G* is a gum-cycle with gum-trees attached.



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 remove its central edge and one other remove an edge from each other block There are $2s \times 3^{b-1}$ spanning trees. This is maximized when s = b.

S 2 3^{b-1}

This argument extends to all block sizes.

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

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New asymptotic results (large v)

Current work by J. Robert Johnson and Mark Walters.

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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 aver-
	age 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)

Brian Cullis and David Butler:

the milling phase of a wheat variety trial has 222 treatments in 28 blocks of size 10. (280 - 222 = 58 and 222 - 58 = 164, so at least 164 treatments must have single replication.)

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subdesign Γ has 82 treatments in 28 blocks of size 5



Whole design Δ has v + bn treatments in b blocks of size k + n; the subdesign Γ has v treatments in b blocks of size k.

New results

Theorem (cf Martin, Chauhan, Eccleston and Chan, 2006; Herzberg and Jarrett, 2007)

The average variance of treatment differences in Δ

= constant \times average variance of treatment differences in Γ + (big constant) \times average variance of block differences in Γ + another constant.

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Consequence

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

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

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.



Youden and Connor chain block design (1953)

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

Youden and Connor

chain block design

(1953)



subdesign is dual of BIBD

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subdesign is dual of BIBD

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



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

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

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