Using graphs to find optimal block designs

R. A. Bailey
University of St Andrews / QMUL (emerita)

Special session for Ching-Shui Cheng,
20 June 2013

Abstract

Ching-Shui Cheng was one of the pioneers of using graph theory to prove results about optimal incomplete-block designs. There are actually two graphs associated with an incomplete-block design, and either can be used.

A block design is D-optimal if it maximizes the number of spanning trees; it is A-optimal if it minimizes the total of the pairwise resistances when the graph is thought of as an electrical network.

I shall report on some surprising results about optimal designs when replication is very low.

Conference on Design of Experiments, Tianjin, June 2006

Problem 1: Factorial design

Problem
There are several treatment factors, with various numbers of levels.
There may not be room to include all combinations of these levels.
There are several inherent factors (also called block factors) on the experimental units.
The inherent factors may pose some constraints on how treatment factors can be applied.
So how do we set about designing the experiment?

Solution
Use Desmond Patterson's design key.

Problem 2: Optimal incomplete-block design

Problem
The design must be in blocks, but each block is too small to contain every treatment.
We want variance to be small, as measured by the D-criterion (minimizing the volume of the ellpsoid of confidence).
How do we set about finding a D-optimal block design?

Solution
Represent the incomplete-block design as a graph (with vertices and edges),
and maximize the number of spanning trees in the graph.

Two papers about the second problem

- Ch'ing Shui Chêng:
  Maximizing the total number of spanning trees in a graph: two related problems in graph theory and optimum design theory.
  Journal of Combinatorial Theory, Series B **31** (1981), 240–248.
- Ching-Shui Cheng:
  Graph and optimum design theories—some connections and examples.
  Bulletin of the International Statistical Institute **49** (1981), part 1, 580–590.

Some early papers

Year	RAB	CSC
1977	factorial (design key)	
1978	factorial (design key)	optimal IBDs
1979		optimal IBDs
1980		optimal IBDs; factorial
1981		optimal IBDs and graphs
1982	factorial	
1984	IBDs	
1985	factorial; IBDs	IBDs and graphs; factorial with trend
1986	IBDs	IBDs
1988		factorial with trend
1989		factorial

Two memorial conferences for R. C. Bose, India, 1988

Calcutta meeting on *Combinatorial Mathematics and Applications*: CSC spoke on “On the optimality of (M.S)-optimal designs in large systems”.

Delhi meeting on *Probability, Statistics and Design of Experiments*: RAB spoke on “Cyclic designs and factorial designs”.

Two joint papers

- C.-S. Cheng and R. A. Bailey:
  Optimality of some two-associate-class partially balanced incomplete-block designs.
  Annals of Statistics **19** (1991), 1667–1671.
- R. A. Bailey, Ching-Shui Cheng and Patricia Kipnis:
  Construction of trend-resistant factorial designs.
  Statistica Sinica **2** (1992), 393–411.

Some later papers and books

Year	RAB	CSC
1993		factorial; optimal IBDs
1995	optimal IBDs	
1998		factorial; BIBDs
1999		factorial
2000		factorial
2001		factorial
2002		factorial
2003		factorial
2004	IBDs	factorial
2005	IBDs	factorial
2006		factorial
2007	optimal IBDs and graphs	
2009	optimal IBDs and graphs	factorial
2011	factorial	factorial
2013	optimal IBDs and graphs	factorial (design key)

With Jo Kunert, Dortmund, April 2009

What makes a block design good for experiments?

I have v treatments that I want to compare.
I have b blocks.
Each block has space for k treatments (not necessarily distinct).

How should I choose a block design?

Two designs with $v = 5$, $b = 7$, $k = 3$: which is better?

Conventions: columns are blocks;
order of treatments within each block is irrelevant;
order of blocks is irrelevant.

binary

1	1	1	1	2	2	2
2	3	3	4	3	3	4
3	4	5	5	4	5	5

non-binary

1	1	1	1	2	2	2
1	3	3	4	3	3	4
2	4	5	5	4	5	5

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

Two designs with $v = 15$, $b = 7$, $k = 3$: which is better?

replications differ by ≤ 1

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

queen-bee design

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

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.

Experimental units and incidence matrix

There are bk experimental units.

If ω is an experimental unit, put

$$\begin{aligned} f(\omega) &= \text{treatment on } \omega \\ g(\omega) &= \text{block containing } \omega. \end{aligned}$$

For $i = 1, \ldots, v$ and $j = 1, \ldots, b$, let

$$n_{ij} = |\{\omega : f(\omega) = i \text{ and } g(\omega) = j\}|$$

$=$ number of experimental units in block j which have treatment i.

The $v \times b$ incidence matrix N has entries n_{ij}.

Levi graph

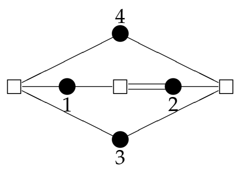
The Levi graph $\tilde{G}$ of a block design Δ has

- one vertex for each treatment,
- one vertex for each block,
- one edge for each experimental unit, with edge ω joining vertex $f(\omega)$ to vertex $g(\omega)$.

It is a bipartite graph,
with n_{ij} edges between treatment-vertex i and block-vertex j.

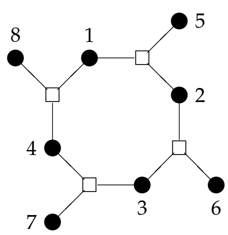
Example 1: $v = 4$, $b = k = 3$

1	2	1
3	3	2
4	4	2



Example 2: $v = 8$, $b = 4$, $k = 3$

1	2	3	4
2	3	4	1
5	6	7	8



Concurrence graph

The concurrence graph G of a block design Δ has

- one vertex for each treatment,
- one edge for each unordered pair α, ω, with $\alpha \neq \omega$, $g(\alpha) = g(\omega)$ and $f(\alpha) \neq f(\omega)$: this edge joins vertices $f(\alpha)$ and $f(\omega)$.

There are no loops.

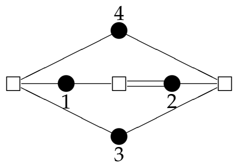
If $i \neq j$ then the number of edges between vertices i and j is

$$\lambda_{ij} = \sum_{s=1}^{b} n_{is} n_{js};$$

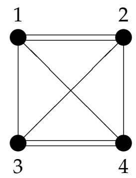
this is called the concurrence of i and j, and is the (i,j)-entry of $\Lambda = NN^\top$.

Example 1: $v = 4$, $b = k = 3$

1	2	1
3	3	2
4	4	2



Levi graph
can recover design
more vertices
more edges if $k = 2$

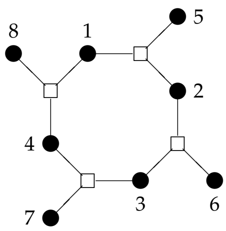


concurrence graph
may have more symmetry

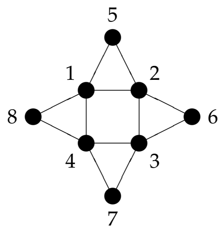
more edges if $k \geq 4$

Example 2: $v = 8$, $b = 4$, $k = 3$

1	2	3	4
2	3	4	1
5	6	7	8



Levi graph



concurrence graph

Laplacian matrices

The Laplacian matrix L of the concurrence graph G is a $v \times v$ matrix with (i,j)-entry as follows:

- if $i \neq j$ then $L_{ij} = -$(number of edges between i and j) $= -\lambda_{ij}$;
- $L_{ii} =$ valency of $i = \sum_{j \neq i} \lambda_{ij}$.

The Laplacian matrix $\tilde{L}$ of the Levi graph $\tilde{G}$ is a $(v+b) \times (v+b)$ matrix with (i,j)-entry as follows:

- $\tilde{L}_{ii} =$ valency of i
$$= \begin{cases} k & \text{if } i \text{ is a block} \\ \text{replication } r_i \text{ of } i & \text{if } i \text{ is a treatment} \end{cases}$$
- if $i \neq j$ then $L_{ij} = -$(number of edges between i and j)
$$= \begin{cases} 0 & \text{if } i \text{ and } j \text{ are both treatments} \\ 0 & \text{if } i \text{ and } j \text{ are both blocks} \\ -n_{ij} & \text{if } i \text{ is a treatment and } j \text{ is a block, or vice versa.} \end{cases}$$

Connectivity

All row-sums of L and of $\tilde{L}$ are zero, so both matrices have 0 as eigenvalue on the appropriate all-1 vector.

Theorem
The following are equivalent.

1. *0 is a simple eigenvalue of L;*
2. *G is a connected graph;*
3. *$\tilde{G}$ is a connected graph;*
4. *0 is a simple eigenvalue of $\tilde{L}$;*
5. *the design Δ is connected in the sense that all differences between treatments can be estimated.*

From now on, assume connectivity.

Call the remaining eigenvalues *non-trivial*. They are all non-negative.

Generalized inverse

Under the assumption of connectivity, the Moore–Penrose generalized inverse L^- of L is defined by

$$L^- = \left(L + \frac{1}{v} J_v \right)^{-1} - \frac{1}{v} J_v,$$

where J_v is the $v \times v$ all-1 matrix.

(The matrix $\frac{1}{v} J_v$ is the orthogonal projector onto the null space of L.)

The Moore–Penrose generalized inverse $\tilde{L}^-$ of $\tilde{L}$ is defined similarly.

Estimation and variance

We measure the response Y_ω on each experimenal unit ω.

If experimental unit ω has treatment i and is in block m ($f(\omega) = i$ and $g(\omega) = m$), then we assume that

$$Y_\omega = \tau_i + \beta_m + \text{random noise}.$$

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.

How do we calculate variance?

Theorem (Standard linear model theory)

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

$$V_{ij} = \left(L^-_{ii} + L^-_{jj} - 2L^-_{ij}\right) k\sigma^2.$$

. . . Or we can use the Levi graph

Theorem

The variance of the best linear unbiased estimator of the simple difference $\tau_i - \tau_j$ is

$$V_{ij} = \left(\tilde{L}^-_{ii} + \tilde{L}^-_{jj} - 2\tilde{L}^-_{ij}\right) \sigma^2.$$

Electrical networks

We can consider the concurrence graph G 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 $1/I$.

Electrical networks: variance

Theorem

The effective resistance R_{ij} between vertices i and j in G is

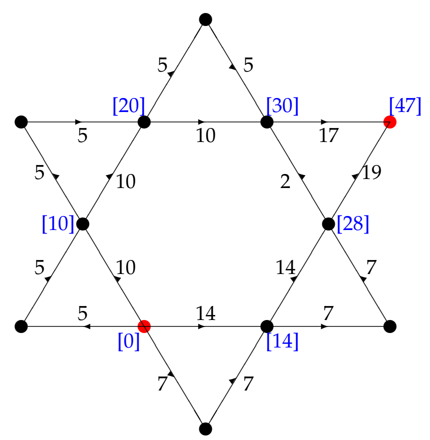
$$R_{ij} = \left(L^-_{ii} + L^-_{jj} - 2L^-_{ij}\right).$$

So

$$V_{ij} = R_{ij} \times k\sigma^2.$$

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

Example calculation: $v = 12$, $b = 6$, $k = 3$



$V = 47$

$I = 36$

$R = \frac{47}{36}$

. . . Or we can use the Levi graph

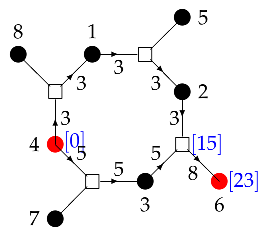
If i and j are treatment vertices in the Levi graph $\tilde{G}$ and $\tilde{R}_{ij}$ is the effective resistance between them in $\tilde{G}$ then

$$V_{ij} = \tilde{R}_{ij} \times \sigma^2.$$

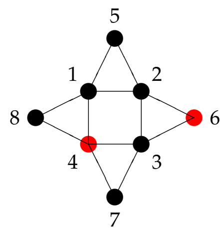
Example 2 yet again: $v = 8$, $b = 4$, $k = 3$

$V = 23 \quad I = 8 \quad R = \frac{23}{8}$

1	2	3	4
2	3	4	1
5	6	7	8



Levi graph



concurrence graph

Average pairwise variance

The variance of the best linear unbiased estimator of the simple difference $\tau_i - \tau_j$ is

$$V_{ij} = \left(L^-_{ii} + L^-_{jj} - 2L^-_{ij}\right) k\sigma^2.$$

Put $\bar{V} =$ average value of the V_{ij}. Then

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

where $\theta_1, \ldots, \theta_{v-1}$ are the nontrivial eigenvalues of L.

Optimality

The design is called

- A-optimal if it minimizes the average of the variances V_{ij}; —equivalently, it maximizes the harmonic mean of the non-trivial eigenvalues of the Laplacian matrix L;
- D-optimal if it minimizes the volume of the confidence ellipsoid for $(\tau_1, \ldots, \tau_v)$; —equivalently, it maximizes the geometric mean of the non-trivial eigenvalues of the Laplacian matrix L;

over all block designs with block size k and the given v and b.

D-optimality: spanning trees

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

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

$$\begin{aligned} &\text{product of non-trivial eigenvalues of } L \\ = {} & v \times \text{number of spanning trees.} \end{aligned}$$

So a design is D-optimal if and only if its concurrence graph G has the maximal number of spanning trees.

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

What about the Levi graph?

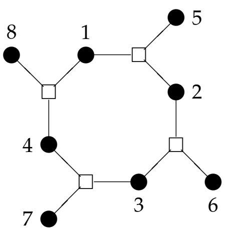
Theorem (Gaffke)
Let G and $\tilde{G}$ be the concurrence graph and Levi graph for a connected incomplete-block design for v treatments in b blocks of size k. Then the number of spanning trees for $\tilde{G}$ is equal to k^{b-v+1} times the number of spanning trees for G.

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

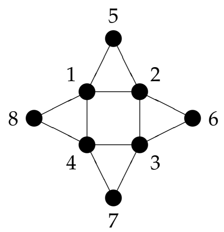
If $v > b$ it is easier to count spanning trees in the Levi graph than in the concurrence graph.

Example 2 one last time: $v = 8$, $b = 4$, $k = 3$

1	2	3	4
2	3	4	1
5	6	7	8

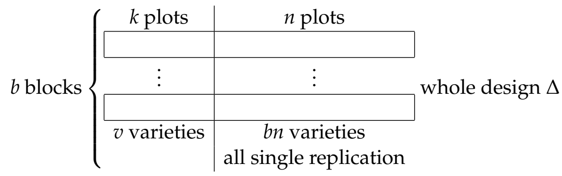


Levi graph
8 spanning trees



concurrence graph
216 spanning trees

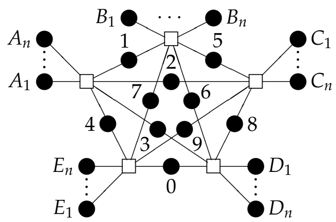
Large blocks; many unreplicated treatments



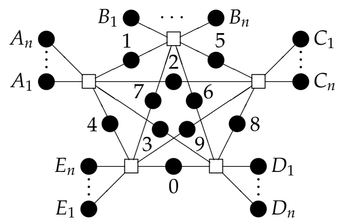
Whole design Δ has $v + bn$ varieties in b blocks of size $k + n$;
the subdesign Γ has v core varieties in b blocks of size k;
call the remaining varieties orphans.

Levi graph: $10 + 5n$ treatments in 5 blocks of $4 + n$ plots

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



Pairwise resistance



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

Sum of the pairwise variances

Theorem (cf Herzberg and Jarrett, 2007)
The sum of the variances of treatment differences in Δ

$$= \textit{constant} + V_1 + nV_3 + n^2V_2,$$

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.)

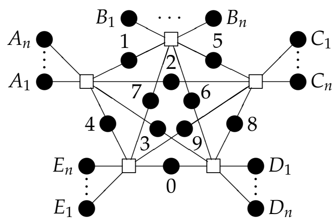
Consequence
For a given choice of k, make Γ as efficient as possible.

A less obvious consequence

Consequence
If n or b is large,
and we want an A-optimal design,
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.

Spanning trees

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



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

D-optimality under very low replication

Consequence

The whole design Δ is D-optimal
for $v + bn$ treatments in b blocks of size $k + n$
if and only if the core design Γ is D-optimal
for v treatments in b blocks of size k.

Consequence

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