Using graphs to find the best block designs

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Abstract

A statistician designing an experiment wants to get as much information as possible from the data gathered. Often this means the most precise estimate possible (that is, an estimate with minimum possible variance) of the unknown parameters. If there are several parameters, this can be interpreted in many ways: do we want to minimize the average variance, or the maximum variance, or the volume of a confidence region for the parameters?

In the case of block designs, these optimality criteria can be calculated from the concurrence graph of the design, and in many cases from its Laplacian eigenvalues. The Levi graph can also be used. The various criteria turn out to be closely connected with other properties of the graph as a network, such as number of spanning trees, isoperimetric number, and the sum of the resistances between pairs of vertices when the graph is regarded as an electrical network.

In this chapter, we discuss the notions of optimality for incomplete-block designs, explain the graph-theoretic connections, and prove some old and new results about optimality.

1 What makes an incomplete-block design good for experiments?

Experiments are designed in many ways: for example, Latin squares, block designs, split-plot designs. Combinatorialists, on the other hand, have a much more specialized usage of the term "design", as we remark later. We are concerned here with incomplete-block designs, more special than the statistician's designs and more general than the mathematician's.

To a statistician, a *block design* has two components. There is an underlying set of experimental units, partitioned into b blocks of size k. There is a further set of v treatments, and also a function f from units to treatments, specifying which treatment is allocated to which experimental unit; that is, $f(\omega)$ is the treatment allocated to experimental unit ω. Thus each block defines a subset, or maybe a multi-subset, of the treatments.

In a *complete-block design*, we have $k = v$ and each treatment occurs once in every block. Here we assume that blocks are *incomplete* in the sense that $k < v$.

We assume that the purpose of the experiment is to find out about the treatments, and differences between them. The blocks are an unavoidable nuisance, an inherent feature of the experimental units. In an agricultural experiment the experimental units may be field plots and the blocks may be fields or plough-lines; in a clinical trial the experimental units may be patients and the blocks hospitals; in process engineering the experimental units may be runs of a machine that is recalibrated each day and the blocks days. See [5] for further examples.

In all of these situations, the values of b, k and v are given. Given these values, not all incomplete-block designs are equally good. This chapter describes some criteria that can be used to choose between them.

For example, Fig. 1 shows two block designs with $v = 15$, $b = 7$ and

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

(a)

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

(b)

Figure 1: Two block designs with $v = 15$, $b = 7$ and $k = 3$

$k = 3$. We use the convention that the treatments are labelled $1, \ldots, v$, that columns represent blocks, and that the order of the entries in each column is not significant. Where necessary, we use the notation Γ_j to refer to the block which is shown as the jth column, for $j = 1, \ldots, b$.

The *replication* r_i of treatment i is defined to be $|f^{-1}(i)|$, which is the number of experimental units to which it is allocated. For the design in Fig. 1(a), $r_i \in \{1, 2\}$ for all i. As we see later, statisticians tend to prefer designs in which all the replications are as equal as possible. If $r_i = r_j$ for $1 \leq i < j \leq v$ then the design is *equireplicate*: then the common value of r_i is usually written as r, and $vr = bk$.

The design in Fig. 1(b) is a *queen-bee design* because there is (at least) one treatment that occurs in every block. Scientists tend to prefer such designs because they have been taught to compare every treatment to one distinguished treatment, which may be called a *control treatment*.

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

(a)

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

(b)

Figure 2: Two block designs with $v = 5$, $b = 7$ and $k = 3$

Fig. 2 shows two block designs with $v = 5$, $b = 7$ and $k = 3$. The design in Fig. 2(b) shows a new feature: treatment 1 occurs on two experimental units in block Γ_1. A block design is *binary* if $f(\alpha) \neq f(\omega)$ whenever α and ω are experimental units in the same block. The design in Fig. 2(a) is binary. It seems to be obvious that binary designs must be better than non-binary ones, but we shall see later that this is not necessarily so. However, if there is any block on which f is constant, then that block provides no information about treatments, so we assume from now on that there are no such blocks.

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

(a)

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

(b)

Figure 3: Two block designs with $v = 7$, $b = 7$ and $k = 3$

Fig. 3 shows two equireplicate binary block designs with $v = 7$, $b = 7$ and $k = 3$. A binary design is *balanced* if every pair of distinct treatments occurs together in the same number of blocks. If that number is λ, then $r(k-1) = (v-1)\lambda$. Such designs are also called 2-*designs* or *BIBDs*. The design in Fig. 3(a) is balanced with $\lambda = 1$; the design in Fig. 3(b) is not balanced.

Pure mathematicians usually assume that, if they exist, balanced designs are better than non-balanced ones. (Indeed, many do not call a structure a 'design' unless it is balanced.) As we shall show in Section 4.1, this assumption is correct for all the criteria considered here. However, for given values of v and k, a non-balanced design with a larger value of b may produce more information than a balanced design with a smaller value of b.

2 Graphs from block designs

2.1 The Levi graph

A simple way of representing a block design is its *Levi graph*, or *incidence graph*, introduced in [40]. This graph has $v + b$ vertices, one for each block and one for each treatment. There are bk edges, one for each experimental unit. If experimental unit ω is in block j and $f(\omega) = i$, then the corresponding edge $\tilde{e}_\omega$ joins vertices i and j. Thus the graph is bipartite, with one part consisting of block vertices and the other part consisting of treatment vertices. Moreover, the graph has multiple edges if the design is not binary. Fig. 4 gives the Levi graph of the design in Fig. 2(b).

We regard two block designs as the same if one can be obtained from the other by permuting the experimental units within each block. Since the vertices of the Levi graph are labelled, there is a bijection between block designs and their Levi graphs.

Let n_{ij} be the number of edges from treatment-vertex i to block-vertex j; that is, treatment i occurs on n_{ij} experimental units in block j. The $v \times b$

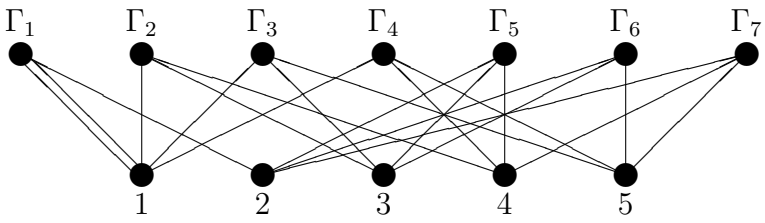


Figure 4: The Levi graph of the design in Fig. 2(b)

matrix $\mathbf{N}$ whose entries are the n_{ij} is the *incidence matrix* of the block design. If the rows and columns of $\mathbf{N}$ are labelled, we can recover the block design from its incidence matrix.

2.2 The concurrence graph

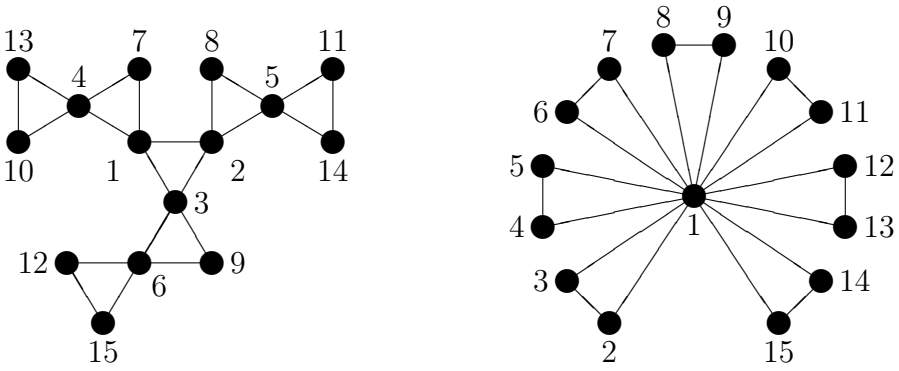
In a binary design, the *concurrence* λ_{ij} of treatments i and j is r_i if $i = j$ and otherwise is the number of blocks in which i and j both occur. For non-binary designs we have to count the number of occurrences of the pair $\{i, j\}$ in blocks according to multiplicity, so that λ_{ij} is the (i, j)-entry of $\mathbf{\Lambda}$, where $\mathbf{\Lambda} = \mathbf{N}\mathbf{N}^\top$. The matrix $\mathbf{\Lambda}$ is called the *concurrence matrix* of the design.

The *concurrence graph* of the design has the treatments as vertices. There are no loops. If $i \neq j$, then there are λ_{ij} edges between vertices i and j. Each such edge corresponds to a pair $\{\alpha, \omega\}$ of experimental units in the same block, with $f(\alpha) = i$ and $f(\omega) = j$: we denote this edge by $e_{\alpha\omega}$. (This edge does not join the experimental units α and ω; it joins the treatments applied to these units.) It follows that the degree d_i of vertex i is given by

$$d_i = \sum_{j \neq i} \lambda_{ij}. \tag{1}$$

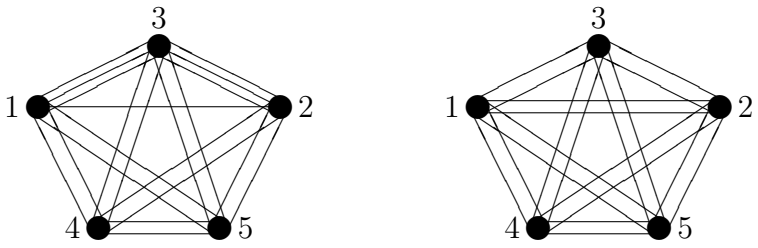
Figs. 5 and 6 show the concurrence graphs of the designs in Figs. 1 and 2, respectively.

If $k = 2$, then the concurrence graph is effectively the same as the block design. Although the block design cannot be recovered from the concurrence graph for larger values of k, we shall see in Section 3.2 that the concurrence graphs contain enough information to decide between two block designs on any of the usual statistical criteria. They were introduced as *variety concurrence graphs* in [44], but are so useful that they may have been considered earlier.



(a) (b)

Figure 5: The concurrence graphs of the designs in Fig. 1



(a) (b)

Figure 6: The concurrence graphs of the designs in Fig. 2

$$\begin{bmatrix} 8 & -1 & -3 & -2 & -2 \\ -1 & 8 & -3 & -2 & -2 \\ -3 & -3 & 10 & -2 & -2 \\ -2 & -2 & -2 & 8 & -2 \\ -2 & -2 & -2 & -2 & 8 \end{bmatrix} \qquad \begin{bmatrix} 8 & -2 & -2 & -2 & -2 \\ -2 & 8 & -2 & -2 & -2 \\ -2 & -2 & 8 & -2 & -2 \\ -2 & -2 & -2 & 8 & -2 \\ -2 & -2 & -2 & -2 & 8 \end{bmatrix}$$

(a) (b)

Table 1: The Laplacian matrices of the concurrence graphs in Fig. 6

2.3 The Laplacian matrix of a graph

Let H be an arbitrary graph with n vertices: it may have multiple edges, but no loops. The *Laplacian matrix* $\mathbf{L}$ of H is defined to be the square matrix with rows and columns indexed by the vertices of H whose (i,i)-entry L_{ii} is the valency of vertex i and whose (i,j)-entry L_{ij} is the negative of the number of edges between vertices i and j if $i \neq j$. Then $L_{ii} = \sum_{j \neq i} L_{ij}$ for $1 \leq i \leq n$, and so the row sums of $\mathbf{L}$ are all zero. It follows that $\mathbf{L}$ has eigenvalue 0 on the all-1 vector; this is called the *trivial eigenvalue* of $\mathbf{L}$. We show below that the multiplicity of the zero eigenvalue is equal to the number of connected components of H. Thus the multiplicity is 1 if and only if H is connected.

Call the remaining eigenvalues of $\mathbf{L}$ *non-trivial*. They are all non-negative, as we show in the following theorem (see [7]).

Theorem 1 *(a) If $\mathbf{L}$ is a Laplacian matrix, then $\mathbf{L}$ is positive semi-definite.*

(b) If $\mathbf{L}$ is a Laplacian matrix of order n and $\mathbf{x}$ is any vector in $\mathbb{R}^n$, then

$$\mathbf{x}^\top \mathbf{L} \mathbf{x} = \sum_{\text{edges } ij} (x_i - x_j)^2.$$

(c) If $\mathbf{L}_1$ and $\mathbf{L}_2$ are the Laplacian matrices of graphs H_1 and H_2 with the same vertices, and if H_2 is obtained from H_1 by inserting one extra edge, then $\mathbf{L}_2 - \mathbf{L}_1$ is positive semi-definite.

(d) If $\mathbf{L}$ is the Laplacian matrix of the graph H, then the multiplicity of the zero eigenvalue of $\mathbf{L}$ is equal to the number of connected components of H.

Proof Each edge between vertices i and j defines a $v \times v$ matrix whose entries are all 0 apart from the following submatrix:

$$\begin{array}{c} \\ i \\ j \end{array} \begin{array}{c} \begin{array}{cc} i & j \end{array} \\ \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \end{array} .$$

The Laplacian is the sum of these matrices, which are all positive semi-definite. This proves (a), (b) and (c).

From (b), the vector $\mathbf{x}$ is in the null space of the Laplacian if and only if $\mathbf{x}$ takes the same value on both vertices of each edge, which happens if and only if it takes a constant value on each connected component. This proves (d). ∎

Theorem 1 shows that the smallest non-trivial eigenvalue of a connected graph is positive. This eigenvalue is sometimes called the *algebraic connectivity* of the graph. The statistical importance of this is shown in Section 3.2.

In Section 3.1 we shall need the Moore–Penrose generalized inverse of $\mathbf{L}^-$ of $\mathbf{L}$ (see [45]). Put $\mathbf{P}_0 = n^{-1}\mathbf{J}_n$, where $\mathbf{J}_n$ is the $n \times n$ matrix whose entries are all 1, so that $\mathbf{P}_0$ is the matrix of orthogonal projection onto the space spanned by the all-1 vector. If H is connected then $\mathbf{L} + \mathbf{P}_0$ is invertible, and

$$\mathbf{L}^- = (\mathbf{L} + \mathbf{P}_0)^{-1} - \mathbf{P}_0,$$

so that $\mathbf{L}\mathbf{L}^- = \mathbf{L}^-\mathbf{L} = \mathbf{I}_n - \mathbf{P}_0$, where $\mathbf{I}_n$ is the identity matrix of order n.

2.4 Laplacians of the concurrence and Levi graphs

There is a relationship between the Laplacian matrices of the concurrence and Levi graphs of a block design Δ. Let $\mathbf{N}$ be the incidence matrix of the design, and $\mathbf{R}$ the diagonal matrix (with rows and columns indexed by treatments) whose (i,i) entry is the replication r_i of treatment i. If the design is equireplicate, then $\mathbf{R} = r\mathbf{I}_v$, where r is the replication number.

For the remainder of the paper, we will use $\mathbf{L}$ for the Laplacian matrix of the concurrence graph G of Δ, and $\tilde{\mathbf{L}}$ for the Laplacian matrix of the Levi graph $\tilde{G}$ of Δ. Then it is straightforward to show that

$$\mathbf{L} = k\mathbf{R} - \mathbf{N}\mathbf{N}^\top, \qquad \tilde{\mathbf{L}} = \begin{bmatrix} \mathbf{R} & -\mathbf{N} \\ -\mathbf{N}^\top & k\mathbf{I} \end{bmatrix}.$$

The Levi graph is connected if and only if the concurrence graph is connected; thus 0 is a simple eigenvalue of $\tilde{\mathbf{L}}$ if and only if it is a simple eigenvalue of $\mathbf{L}$, which in turn occurs if and only if all contrasts between treatment parameters are estimable (see Section 3.1). A block design with this property is itself called *connected*: we consider only connected block designs.

In the equireplicate case, the above expressions for $\mathbf{L}$ and $\tilde{\mathbf{L}}$ give a relationship between their Laplacian eigenvalues, as follows. Let $\mathbf{x}$ be an eigenvector of $\mathbf{L}$ with eigenvalue $\phi \neq rk$. Then, for each of the two solutions θ of the quadratic equation

$$rk - \phi = (r - \theta)(k - \theta),$$

there is a unique vector $\mathbf{z}$ in $\mathbb{R}^b$ such that $[\ \mathbf{x}^\top \quad \mathbf{z}^\top\ ]^\top$ is an eigenvector of $\tilde{\mathbf{L}}$ with eigenvalue θ. Conversely, any eigenvalue $\theta \neq k$ of $\tilde{\mathbf{L}}$ arises in this way.

The Laplacian matrices of the concurrence graphs in Fig. 6 are shown in Table 1.

3 Statistical issues

3.1 Estimation and variance

As part of the experiment, we measure the response Y_ω on each experimental unit ω. If ω is in block Γ, then we assume that

$$Y_\omega = \tau_{f(\omega)} + \beta_\Gamma + \varepsilon_\omega; \tag{2}$$

here, τ_i is a constant depending on treatment i, β_Γ is a constant depending on block Γ, and ε_ω is a random variable with expectation 0 and variance σ^2. Furthermore, if $\alpha \neq \omega$, then ε_α and ε_ω are uncorrelated.

It is clear that we can add a constant to every block parameter, and subtract that constant from every treatment parameter, without changing (2). It is therefore impossible to estimate the individual treatment parameters. However, if the design is connected, then we can estimate all *contrasts* in the treatment parameters: that is, all linear combinations of the form $\sum_i x_i\tau_i$ for which $\sum_i x_i = 0$. In particular, we can estimate all the simple treatment differences $\tau_i - \tau_j$.

An *estimator* is a function of the responses Y_ω, so it is itself a random variable. An estimator of a value is *unbiased* if its expectation is equal to the true value; it is *linear* if it is a linear function of the responses. Amongst linear unbiased estimators, the *best* one (the so-called BLUE), is the one with the least variance. Let V_{ij} be the variance of the BLUE for $\tau_i - \tau_j$.

If all the experimental units form a single block, then the BLUE of $\tau_1 - \tau_2$ is just the difference between the average responses for treatments 1 and 2. It follows that

$$V_{12} = \left(\frac{1}{r_1} + \frac{1}{r_2}\right)\sigma^2.$$

When $v = 2$, this variance is minimized (for a given number of experimental units) when $r_1 = r_2$. Moreover, if the responses are normally distributed then the length of the 95% confidence interval for $\tau_1 - \tau_2$ is proportional to $\mathrm{t}(r_1 + r_2 - 2, 0.975)\sqrt{V_{12}}$, where $\mathrm{t}(d, p)$ is the $100p$-th percentile of the t distribution on d degrees of freedom. The smaller the confidence interval, the more likely is our estimate to be close to the true value. This length can be made smaller by increasing $r_1 + r_2$, decreasing $|r_1 - r_2|$, or decreasing σ^2.

However, matters are not so simple when $k < v$ and $v > 2$. The following result can be found in any statistical textbook about block designs (see the section on further reading for recommendations).

Theorem 2 *Let* $\mathbf{L}$ *be the Laplacian matrix of the concurrence graph of a connected block design. If* $\sum_i x_i = 0$*, then the variance of the BLUE of*

$\sum_i x_i\tau_i$ *is equal to* $(\mathbf{x}^\top \mathbf{L}^- \mathbf{x})k\sigma^2$. *In particular, the variance* V_{ij} *of the BLUE of the simple difference* $\tau_i - \tau_j$ *is given by* $V_{ij} = \left(L_{ii}^- + L_{jj}^- - 2L_{ij}^-\right) k\sigma^2$.

3.2 Optimality criteria

We want all of the V_{ij} to be as small as possible, but this is a multi-dimensional problem if $v > 2$. Let $\bar{V}$ be the average of the variances V_{ij} over all treatments i, j with $i \neq j$. Theorem 2 shows that, for each fixed i,

$$\begin{aligned}\sum_{j\neq i} V_{ij} &= \sum_{j\neq i}(L_{ii}^- + L_{jj}^- - 2L_{ij}^-)k\sigma^2 \\ &= [(v-1)L_{ii}^- + (\mathrm{Tr}(\mathbf{L}^-) - L_{ii}^-) + 2L_{ii}^-]k\sigma^2 \\ &= [vL_{ii}^- + \mathrm{Tr}(\mathbf{L}^-)]k\sigma^2,\end{aligned}$$

because the row sums and column sums of L are all 0. It follows that $\bar{V} = 2k\sigma^2 \,\mathrm{Tr}(\mathbf{L}^-)/(v-1)$.

Let $\theta_1, \ldots, \theta_{v-1}$ be the non-trivial eigenvalues of $\mathbf{L}$, now listed according to multiplicity and in non-decreasing order. Then

$$\mathrm{Tr}(\mathbf{L}^-) = \frac{1}{\theta_1} + \cdots + \frac{1}{\theta_{v-1}},$$

and so

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

A block design is defined to be *A-optimal* (in some given class of designs with the same values of b, k and v) if it minimizes the value of $\bar{V}$; here 'A' stands for 'average'. Thus a design is A-optimal if and only if it maximizes the harmonic mean of $\theta_1, \ldots, \theta_{v-1}$.

For $v > 2$, the generalization of a confidence interval is a confidence ellipsoid centered at the point $(\hat{\tau}_1, \ldots, \hat{\tau}_v)$ which gives the estimated value of $(\tau_1, \ldots, \tau_v)$ in the $(v-1)$-dimensional subspace of $\mathbb{R}^v$ for which $\sum \tau_i = 0$. A block design is called *D-optimal* if it minimizes the volume of this confidence ellipsoid. Since this volume is proportional to $\sqrt{\det(\mathbf{L}^- + \mathbf{P}_0)}$, a design is D-optimal if and only if it maximizes the geometric mean of $\theta_1, \ldots, \theta_{v-1}$. Here 'D' stands for 'determinant'.

Rather than looking at averages, we might consider the worst case. If all the entries in the vector $\mathbf{x}$ are multiplied by a constant c, then the variance of the estimator of $\sum x_i\tau_i$ is multiplied by c^2. Thus, those contrast vectors $\mathbf{x}$ which give the largest variance relative to their own length are those which maximize $\mathbf{x}^\top \mathbf{L}^- \mathbf{x}/\mathbf{x}^\top \mathbf{x}$; these are precisely the eigenvectors of $\mathbf{L}$ with eigenvalue θ_1. A design is defined to be *E-optimal* if it maximizes the value of θ_1; here 'E' stands for 'extreme'.

More generally, for p in $(0, \infty)$, a design is called Φ_p-*optimal* if it minimizes

$$\left(\frac{\sum_{i=1}^{v-1} \theta_i^{-p}}{v-1} \right)^{1/p}.$$

Thus A-optimality corresponds to $p = 1$, D-optimality corresponds to the limit as $p \to 0$, and E-optimality corresponds to the limit as $p \to \infty$.

Let $\mathbf{L}_1$ and $\mathbf{L}_2$ be the Laplacian matrices of the concurrence graphs of block designs Δ_1 and Δ_2 for v treatments in blocks of size k. If $\mathbf{L}_2 - \mathbf{L}_1$ is positive semi-definite, then Δ_2 is at least as good as Δ_1 on all the Φ_p-criteria. Theorem 1(c) shows that adding an extra block to a design cannot decrease its performance on any Φ_p-criterion.

There are even more general classes of optimality criteria (see [28] and [48] for details). Here we concentrate on A-, D- and E-optimality.

3.3 Questions and an example

A first obvious question to ask is: do these criteria agree with each other?

Our optimality properties are all functions of the concurrence graph. What features of this graph should we look for if we are searching for optimal, or near-optimal, designs? Symmetry? (Nearly) equal degrees? (Nearly) equal numbers of edges between pairs of vertices? Distance-regularity? Large girth (ignoring cycles within a block)? Small numbers of short cycles (ditto)? High connectivity? Non-trivial automorphism group?

Is it more useful to look at the Levi graph rather than the concurrence graph?

Example 1 Fig. 7 shows the values of the A- and D-criteria for all equireplicate block designs with $v = 8$, $b = 12$ and $k = 2$: of course, these are just regular graphs with 8 vertices and degree 3. The harmonic mean is shown on the A-axis, and the geometric mean on the D-axis. (Note that this figure includes some designs that were omitted from Figure 3 of [4].) The rankings on these two criteria are not exactly the same, but they do agree at the top end, where it matters. The second-best graph on both criteria is the cube; the best is the Möbius ladder, whose vertices are the elements of $\mathbb{Z}_8$ and whose edges are $\{i, i+1\}$ and $\{i, i+4\}$ for i in $\mathbb{Z}_8$. These two graphs are so close on both criteria that, for practical purposes, they can be regarded as equally good.

The plotting symbols show the edge-connectivity of the graphs: edge-connectivity 3, 2, 1 is shown as $\times$, $+$, $\circ$ respectively. This does suggest that the higher the edge-connectivity the better is the design on the A- and D-

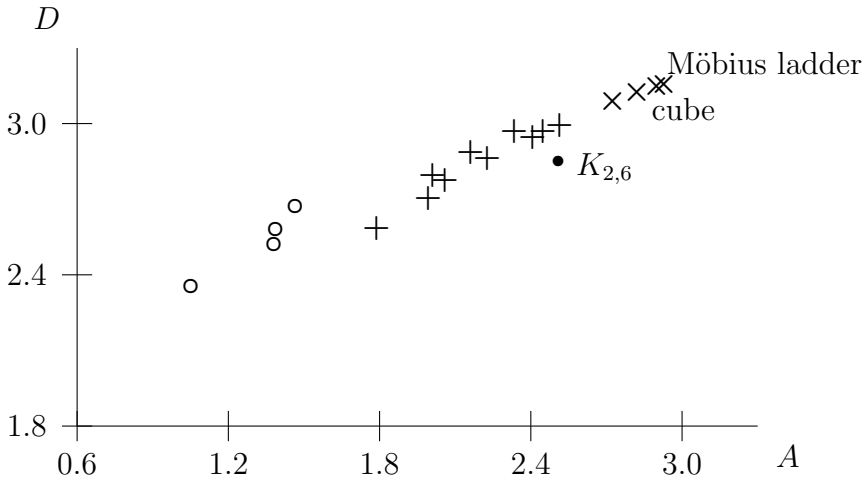


Figure 7: Values of two optimality criteria for all equireplicate block designs with $v = 8$, $b = 12$, and $k = 2$, and for $K_{2,6}$

criteria. This is intuitively reasonable: if $k = 2$, then the edge-connectivity is the minimum number of blocks whose removal disconnects the design. In this context, it has been called *breakdown number*: see [39].

The four graphs with edge-connectivity 3 have no double edges, so concurrences differ by at most 1. The only other regular graph with no double edges is ranked eighth (amongst regular graphs) by the A-criterion. This suggests that (near-)equality of concurrences is not sufficient to give a good design.

The symbol • shows the non-regular graph $K_{2,6}$, which also has eight vertices and twelve edges. It is not as good as the regular graphs with edge-connectivity 3, but it beats many of the other regular graphs.

This pattern is typical of the block designs investigated by statisticians for most of the 20th century. The A- and D-criteria agree closely at the top end. High edge-connectivity appears to show good designs. Many of the best designs have a high degree of symmetry.

4 Highly patterned block designs

4.1 Balanced incomplete-block designs

BIBDs are intuitively appealing, as they seem to give equal weight to all treatment comparisons. They were introduced for agricultural experiments

by Yates in [54].

In [38], Kshirsagar proved that, if there exists a BIBD for given values of v, b and k, then it is A-optimal. Kiefer generalized this in [35] to cover Φ_p-optimality for all p in $(0, \infty)$, including the limiting cases of D- and E-optimality. The core of Kiefer's proof is as follows: binary designs maximize $\mathrm{Tr}(\mathbf{L})$, which is equal to $\sum_{i=1}^{v-1} \theta_i$; for any fixed value T of this sum of positive numbers, $\sum \theta_i^{-p}$ is minimized at $[T/(v-1)]^{-p}$ when $\theta_1 = \cdots = \theta_{v-1} = T/(v-1)$; and T^{-p} is minimized when T is maximized.

4.2 Other special designs

Of course, it frequently occurs that the values of b, v, k available for an experiment are such that no BIBD exists. (Necessary conditions for the existence of a BIBD include the well-known divisibility conditions $v \mid bk$ and $v(v-1) \mid bk(k-1)$, which follow from the elementary results in Section 1, and *Fisher's inequality* asserting that $b \geq v$.)

In the absence of a BIBD, various other special types of design have been considered, and some of these have been proved optimal. Here is a short sample.

A design is *group-divisible* if the treatments can be partitioned into "groups" all of the same size, so that the number of blocks containing two treatments is λ_1 if they belong to the same group and λ_2 otherwise. Chêng [16, 17] showed that if there is a group-divisible design with two groups and $\lambda_2 = \lambda_1 + 1$ in the class of designs with given v, b, k, then it is Φ_p-optimal for all p, and in particular is A-, D- and E-optimal.

A *regular-graph design* is a binary equireplicate design with two possible concurrences λ and $\lambda+1$. It is easily proved that, in such a design, the number of treatments lying in $\lambda+1$ blocks with a given treatment is constant; so the graph H whose vertices are the treatments, two vertices joined if they lie in $\lambda+1$ blocks, is regular.

Now Chêng [17] showed that a group-divisible design with $\lambda_2 = \lambda_1 + 1 = 1$, if one exists, is Φ_p-optimal in the class of regular-graph designs for all p. Cheng and Bailey [20] showed that a regular-graph design for which the graph is *strongly regular* (see [15]) and which has singular concurrence matrix is Φ_p-optimal, for all p, among binary equireplicate designs with given v, b, k.

Designs with the property described here are particular examples of *partially balanced designs* with respect to an association scheme: see Bailey [3].

Another class which has turns out to be optimal in many cases, but whose definition is less combinatorial, consists of the *variance-balanced designs*, which we consider later in the chapter.

5 Graph concepts linked to D-optimality

5.1 Spanning trees of the concurrence graph

Let G be the concurrence graph of a connected block design, and let $\mathbf{L}$ be its Laplacian matrix. A *spanning tree* for G is a spanning subgraph which is a tree. Kirchhoff's famous Matrix-tree theorem in [36] states the following:

Theorem 3 *If G is a connected graph with v vertices and Laplacian matrix $\mathbf{L}$, then the product of the non-trivial eigenvalues of $\mathbf{L}$ is equal to v multiplied by the number of spanning trees for G.*

Thus we have a test for D-optimality:

> *A design is D-optimal if and only if its concurrence graph has the maximal number of spanning trees.*

Note that Theorem 3 gives an easy proof of Cayley's theorem on the number of spanning trees for the complete graph K_v. The non-trivial eigenvalues of its Laplacian matrix are all equal to v, so Theorem 3 shows that it has v^{v-2} spanning trees.

If G is sparse, it may be much easier to count the number of spanning trees than to compute the eigenvalues of $\mathbf{L}$. For example, if G has a single cycle, which has length s, then the number of spanning trees is s, irrespective of the remaining edges in G.

In the context of optimal block designs, Gaffke discovered the importance of Kirchhoff's theorem in [26]. Cheng followed this up in papers such as [16, 17, 19]. Particularly intriguing is the following theorem from [21].

Theorem 4 *Consider block designs with $k = 2$ (connected graphs). For each given v there is a threshold b_0 such that if $b \geq b_0$ then any D-optimal design for v treatments in b blocks of size 2 is* nearly balanced *in the sense that*

- *no pair of replications differ by more than 1;*
- *for each fixed i, no pair of concurrences λ_{ij} differ by more than 1.*

In fact, there is no known example with $b_0 > v - 1$, which is the minimal number of blocks required for connectivity.

5.2 Spanning trees of the Levi graph

In [27] Gaffke stated the following relationship between the numbers of spanning trees in the concurrence graph and the Levi graph.

Theorem 5 *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.*

Thus, an alternative test for D-optimality is to count the number of spanning trees in the Levi graph. For binary designs, the Levi graph has fewer edges than the concurrence graph if and only if $k \geq 4$.

6 Graph concepts linked to A-optimality

6.1 The concurrence graph as an electrical network

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. Then current flows in the network, according to these rules.

Ohm's Law: In every edge, the voltage drop is the product of the current and the resistance.

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.

Kirchhoff's Current Law: At each vertex which is not connected to the battery, the total current coming in is equal to the total current going out.

We find the total current from i to j, and then use Ohm's Law to define the effective resistance R_{ij} between i and j as the reciprocal of this current. It is a standard result of electrical network theory that the linear equations implicitly defined above for the currents and voltage differences have a unique solution.

Let $\mathcal{T}$ be the set of treatments and Ω the set of experimental units. Current flows in each edge $e_{\alpha\omega}$, where α and ω are experimental units in the same block which receive different treatments; let $I(\alpha, \omega)$ be the current from $f(\alpha)$ to $f(\omega)$ in this edge. Thus I is a function $I: \Omega \times \Omega \mapsto \mathbb{R}$ such that

(a) $I(\alpha, \omega) = 0$ if $\alpha = \omega$ or if $f(\alpha) = f(\omega)$ or if α and ω are in different blocks.

(b) $I(\alpha, \omega) = -I(\omega, \alpha)$ for (α, ω) in $\Omega \times \Omega$.

This defines a further function $I_{\text{out}}: \mathcal{T} \mapsto \mathbb{R}$ by

$$I_{\text{out}}(l) = \sum_{\alpha: f(\alpha)=l} \sum_{\omega \in \Omega} I(\alpha, \omega) \quad \text{for } l \text{ in } \mathcal{T}.$$

Voltage is another function $V: \mathcal{T} \mapsto \mathbb{R}$. The following two conditions ensure that Ohm's and Kirchhoff's Laws are satisfied.

(c) If there is any edge in G between $f(\alpha)$ and $f(\omega)$, then

$$I(\alpha, \omega) = V(f(\alpha)) - V(f(\omega)).$$

(d) If $l \notin \{i, j\}$, then $I_{\text{out}}(l) = 0$.

If G is connected and different voltages $V(i)$ and $V(j)$ are given for a pair of distinct treatments i and j, then there are unique functions I and V satisfying conditions (a)–(d). Moreover, $I_{\text{out}}(j) = -I_{\text{out}}(i) \neq 0$. Then R_{ij} is defined by

$$R_{ij} = \frac{V(i) - V(j)}{I_{\text{out}}(i)}.$$

It can be shown that the value of R_{ij} does not depend on the choice of values for $V(i)$ and $V(j)$, so long as these are different. In practical examples, it is usually convenient to take $V(i) = 0$ and let I take integer values.

What has all of this got to do with block designs? The following theorem, which is a standard result from electrical engineering, gives the answer.

Theorem 6 *If* $\mathbf{L}$ *is the Laplacian matrix of a connected graph* G*, then the effective resistance* R_{ij} *between vertices* i *and* j *is given by*

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

Comparing this with Theorem 2, we see that $V_{ij} = R_{ij} \times k\sigma^2$. Hence we have a test for A-optimality:

> *A design is A-optimal if and only if its concurrence graph, regarded as an electrical network, minimizes the sum of the pairwise effective resistances between all pairs of vertices.*

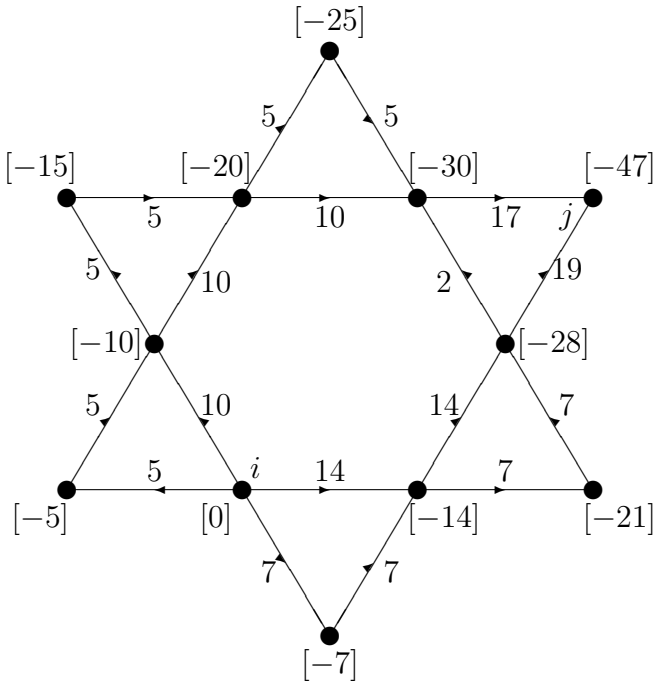


Figure 8: The current between vertices i and j in a concurrence graph

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

Figure 8 shows the concurrence graph of a block design with $v = 12$, $b = 6$ and $k = 3$. Only vertices i and j are labelled. Otherwise, numbers beside arrows denote current and numbers in square brackets denote voltage. It is straightforward to check that conditions (a)–(d) are satisfied. Now $V(i) - V(j) = 47$ and $I_{\text{out}}(i) = 36$, and so $R_{ij} = 47/36$. Therefore $V_{ij} = (47/12)\sigma^2$. Moreover, for graphs consisting of b triangles arranged in a cycle like this, it is clear that average effective resistance, and hence the average pairwise variance, can be calculated as a function of b.

6.2 The Levi graph as an electrical network

The Levi graph $\tilde{G}$ of a block design can also be considered as an electrical network. Denote by $\mathcal{B}$ the set of blocks. Now current is defined on the ordered edges of the Levi graph. Recall that, if ω is an experimental unit in block Γ, then the edge $\tilde{e}_\omega$ joins Γ to $f(\omega)$. Thus current is defined on $(\Omega \times \mathcal{B}) \cup (\mathcal{B} \times \Omega)$ and voltage is defined on $\mathcal{T} \cup \mathcal{B}$. Conditions (a)–(d) in Section 6.1 need to be modified appropriately.

The next theorem shows that a current–voltage pair (I, V) on the concurrence graph G can be transformed into a current–voltage pair $(\tilde{I}, \tilde{V})$ on

the Levi graph $\tilde{G}$. In $\tilde{G}$, the current $\tilde{I}(\alpha, \Gamma)$ flows in edge $\tilde{e}_\alpha$ from vertex $f(\alpha)$ to vertex Γ, where $\alpha \in \Gamma$. Hence the pairwise variance V_{ij} can also be calculated from the effective resistance $\tilde{R}_{ij}$ in the Levi graph.

Theorem 7 *Let G be the concurrence graph and $\tilde{G}$ be the Levi graph of a connected block design with block size k. If i and j are two distinct treatments, let R_{ij} and $\tilde{R}_{ij}$ be the effective resistance between vertices i and j in the electrical networks defined by G and $\tilde{G}$, respectively. Then $\tilde{R}_{ij} = kR_{ij}$, and so $V_{ij} = \tilde{R}_{ij}\sigma^2$.*

Proof Let (I, V) be a current–voltage pair on G. For $(\alpha, \Gamma) \in \Omega \times \mathcal{B}$, put

$$\tilde{I}(\alpha, \Gamma) = -\tilde{I}(\Gamma, \alpha) = \sum_{\omega \in \Gamma} I(\alpha, \omega)$$

if $\alpha \in \Gamma$; otherwise, put $\tilde{I}(\alpha, \Gamma) = \tilde{I}(\Gamma, \alpha) = 0$. Put $\tilde{V}(i) = kV(i)$ for all i in $\mathcal{T}$, and

$$\tilde{V}(\Gamma) = \sum_{\omega \in \Gamma} V(f(\omega))$$

for all Γ in $\mathcal{B}$. It is clear that $\tilde{I}$ satisfies the analogues of conditions (a) and (b).

If $\alpha \in \Gamma$, then

$$\begin{aligned} \tilde{I}(\alpha, \Gamma) &= \sum_{\omega \in \Gamma} I(\alpha, \omega) \\ &= \sum_{\omega \in \Gamma} [V(f(\alpha)) - V(f(\omega))] \\ &= kV(f(\alpha)) - \tilde{V}(\Gamma) = \tilde{V}(f(\alpha)) - \tilde{V}(\Gamma), \end{aligned}$$

so the analogue of condition (c) is satisfied.

If $\Gamma \in \mathcal{B}$, then

$$\tilde{I}_{\text{out}}(\Gamma) = \sum_{\alpha \in \Gamma} \tilde{I}(\Gamma, \alpha) = -\sum_{\alpha \in \Gamma} \sum_{\omega \in \Gamma} I(\alpha, \omega) = 0,$$

because $I(\alpha, \alpha) = 0$ and $I(\alpha, \omega) = -I(\omega, \alpha)$. If $l \in \mathcal{T}$ then

$$\tilde{I}_{\text{out}}(l) = \sum_{\alpha : f(\alpha) = l} \sum_{\Gamma \in \mathcal{B}} \tilde{I}(\alpha, \Gamma) = \sum_{\alpha : f(\alpha) = l} \sum_{\omega \in \Omega} I(\alpha, \omega) = I_{\text{out}}(l).$$

In particular, $\tilde{I}_{\text{out}}(l) = 0$ if $l \notin \{i, j\}$, which shows that the analogue of condition (d) is satisfied. It follows that $(\tilde{I}, \tilde{V})$ is the current–voltage pair on $\tilde{G}$ defined by $\tilde{V}(i)$ and $\tilde{V}(j)$.

Now

$$\tilde{R}_{ij} = \frac{\tilde{V}(i) - \tilde{V}(j)}{\tilde{I}_{\text{out}}(i)} = \frac{k(V(i) - V(j))}{I_{\text{out}}(i)} = kR_{ij}.$$

Then Theorems 2 and 6 show that $V_{ij} = R_{ij}\sigma^2$. ∎

When $k = 2$ it seems to be easier to use the concurrence graph than the Levi graph, because it has fewer vertices, but for larger values of k the Levi graph may be better, as it does not have all the within-block cycles that the concurrence graph has. Fig. 9 gives the Levi graph of the block design whose concurrence graph is in Fig. 8, with the same two vertices i and j attached to the battery. This gives $\tilde{R}_{ij} = 47/12$, which is in accordance with Theorem 7.

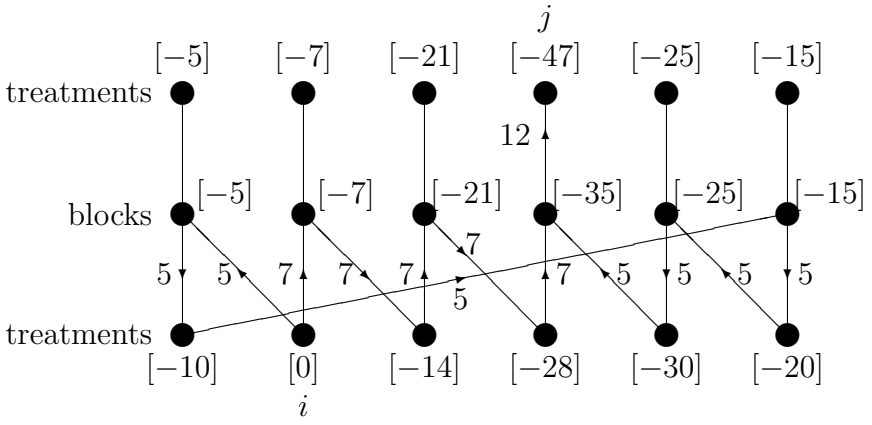


Figure 9: Current between i and j for the Levi graph corresponding to the concurrence graph in Fig. 8

Here is another way of visualizing Theorem 7. From the block design we construct a graph G_0 with vertex-set $\mathcal{T} \cup \Omega \cup \mathcal{B}$: the edges are $\{\alpha, \Gamma\}$ for $\alpha \in \Gamma \in \mathcal{B}$ and $\{\alpha, f(\alpha)\}$ for $\alpha \in \Omega$. Let (I_0, V_0) be a current–voltage pair on G_0 for which both battery vertices are in $\mathcal{T}$. We obtain the Levi graph $\tilde{G}$ from G_0 by becoming blind to the vertices in Ω. Thus the resistance in each edge of $\tilde{G}$ is twice that in each edge in G_0, so this step multiplies each effective resistance by 2.

Because none of the battery vertices is in $\mathcal{B}$, we can now obtain G from $\tilde{G}$ by replacing each path of the form (i, Γ, j) by an edge (i, j). There is no harm in scaling all the voltages by the same amount, so we can obtain (I, V) on G from $(\tilde{I}, \tilde{V})$ on $\tilde{G}$ by putting $V(i) = \tilde{V}(i)/k$ for i in $\mathcal{T}$, and $I(\alpha, \omega) = V(f(\alpha)) - V(f(\omega))$ for α, ω in the same block. If Γ is a block, then

$$0 = \sum_{\alpha \in \Gamma} \tilde{I}(\alpha, \Gamma) = \sum_{\alpha \in \Gamma} [\tilde{V}(f(\alpha)) - \tilde{V}(\Gamma)] = k \sum_{\alpha \in \Gamma} V(f(\alpha)) - k\tilde{V}(\Gamma),$$

and so $\tilde{V}(\Gamma) = \sum_{\alpha\in\Gamma} V(f(\alpha))$. Also, if $\alpha \in \Gamma$, then

$$\begin{aligned}\sum_{\omega\in\Gamma} I(\alpha,\omega) &= \sum_{\omega\in\Gamma}[V(f(\alpha)) - V(f(\omega))] \\ &= kV(f(\alpha)) - \sum_{\omega\in\Gamma} V(f(\omega)) \\ &= \tilde{V}(f(\alpha)) - \tilde{V}(\Gamma) \\ &= \tilde{I}(\alpha,\Gamma).\end{aligned}$$

Therefore, this transformation reverses the one used in the proof of Theorem 7.

There is yet another way of obtaining Theorem 7. If we use the responses Y_ω to estimate the block parameters β_Γ in (2) as well as the treatment parameters τ_i, then standard theory of linear models shows that, if the design is connected, then we can estimate linear combinations of the form $\sum_{i=1}^{v} x_i\tau_i + \sum_{j=1}^{b} z_j\beta_j$ so long as $\sum x_i = \sum z_j$. Moreover, the variance of the BLUE of this linear combination is

$$[\ \mathbf{x}^\top \quad \mathbf{z}^\top\ ]\mathbf{C}^- \begin{bmatrix}\mathbf{x}\\ \mathbf{z}\end{bmatrix}\sigma^2, \qquad \text{where} \qquad \mathbf{C} = \begin{bmatrix}\mathbf{R} & \mathbf{N}\\ \mathbf{N}^\top & k\mathbf{I}_b\end{bmatrix}$$

and $\mathbf{R}$ is the diagonal matrix of replications.

If we reparametrize equation (2) by replacing β_j by $-\gamma_j$ for $j = 1, \ldots, b$, then the estimable quantities are the contrasts in $\tau_1, \ldots, \tau_v, \gamma_1, \ldots, \gamma_b$. The so-called *information matrix* $\mathbf{C}$ must be modified by multiplying the last b rows and the last b columns by -1: this gives precisely the Laplacian $\tilde{\mathbf{L}}$ of the Levi graph $\tilde{G}$. Just as for $\mathbf{L}$, but unlike $\mathbf{C}$, the null space is spanned by the all-1 vector.

6.3 Spanning thickets

We have seen that the value of the D-criterion is a function of the number of spanning trees of the concurrence graph G. It turns out that the closely related notion of a spanning thicket enables us to calculate the A-criterion; more precisely, the value of each pairwise effective resistance in G.

A *spanning thicket* for the graph is a spanning subgraph that consists of two trees (one of them may be an isolated vertex).

Theorem 8 *If i and j are distinct vertices of G then*

$$R_{ij} = \frac{\text{number of spanning thickets with } i,\ j \text{ in different parts}}{\text{number of spanning trees}}\ .$$

This is also rather easy to calculate directly when the graph is sparse.

Summing all the R_{ij} and using Theorem 8 gives the following result from [49].

Theorem 9 *If F is a spanning thicket for the concurrence graph G, denote by F_1 and F_2 the sets of vertices in its two trees. Then*

$$\sum_{i<j} R_{ij} = \frac{\sum_{\text{spanning thickets } F} |F_1|\,|F_2|}{\text{number of spanning trees}}$$

6.4 Random walks and electrical networks

It was first pointed out by Kakutani in 1945 that there is a very close connection between random walks and electrical networks. In a simple random walk, a single step works as follows: starting at a vertex, we choose an edge containing the vertex at random, and move along it to the other end. This definition accommodates multiple edges, and is easily adapted to graphs with edge weights (where the probability of moving along an edge is proportional to the weight of the edge).

If we are thinking of an edge-weighted graph as an electrical network, we take the weights to be the conductances of the edges (the reciprocals of the resistances).

The connection is simple to state:

Theorem 10 *Let i and j be distinct vertices of the connected edge-weighted graph G. Apply voltages of 1 at i and 0 at j. Then the voltage at a vertex l is equal to the probability that the random walk, starting at l, reaches i before it reaches j.*

From this theorem, it is possible to derive a formula for the effective resistance between two vertices. Here are two such formulas. Given two vertices i and j, let $P_{\text{esc}}(i \to j)$ be the probability that a random walk starting at i reaches j before returning to i; and let $S_i(i,j)$ be the expected number of times that a random walk starting at i visits i before reaching j. Then the effective resistance between i and j is given by either of the two expressions

$$\frac{1}{d_i P_{\text{esc}}(i \to j)} \qquad \text{and} \qquad \frac{S_i(i,j)}{d_i},$$

where d_i is the degree of i. (If the edge resistances are not all 1, then the term d_i should be replaced by the sum of the reciprocals of the resistances of all edges incident with vertex i.)

The random walk approach gives alternative proofs of some of the main results about electrical networks. We discuss this further in the guide to the literature.

6.5 Foster's formula and generalizations

In 1948, Foster [25] discovered that the sum of the effective resistances between all *adjacent* pairs of vertices of a connected graph on v vertices is equal to $v-1$. Thirteen years later, he found a similar formula for pairs of vertices at distance 2:

$$\sum_{i\sim h\sim j} \frac{R_{ij}}{d_h} = v - 2.$$

Further extensions have been found, but require a stronger condition on the graph. The sum of resistances between all pairs of vertices at distance at most m can be written down explicitly if the graph is *walk-regular up to distance* m; this means that the number of closed walks of length k starting and finishing at a vertex i is independent of i, for $k \leq m$. The formula was discovered by Emil Vaughan, to whom this part of the chapter owes a debt.

In particular, if the graph is distance-regular (see [14]), then the value of the A-criterion can be written down in terms of the so-called *intersection array* of the graph.

6.6 Distance

At first sight it seems obvious that pairwise variance should decrease as concurrence increases, but there are many counter-examples to this. However, the following theorem is proved in [3].

Theorem 11 *If the Laplacian matrix* $\mathbf{L}$ *has precisely two distinct non-trivial eigenvalues, then pairwise variance is a decreasing linear function of concurrence.*

It does appear that effective resistance, and hence pairwise variance, generally increases with distance in the concurrence graph. In [7, Question 5.1] we pointed out that this is not always exactly so, and asked if it is nevertheless true that the maximal value of R_{ij} is achieved for some pair of vertices $\{i, j\}$ whose distance apart in the graph is maximal. Here is a counter-example.

Example 2 Let $k = 2$, so that the block design is the same as its concurrence graph. Take $v = 10$ and $b = 14$. The graph consists of a cube, with two extra vertices 1 and 2 attached as leaves to vertex 3. The vertex antipodal

to 3 in the cube is labelled 4. It is straightforward to check (either using an electrical network, or by using the fact that the cube is distance-regular) that the effective resistance between a pair of cube vertices is 7/12, 3/4 and 5/6 for vertices at distances 1, 2 and 3. Hence $R_{1j} \leq 11/6$ for all cube vertices j, while $R_{12} = 2$. On the other hand, the distance between vertices 1 and 2 is only 2, while that between either of them and vertex 4 is 4.

There are some 'nice' graphs where pairwise variance does indeed increase with distance. The following result is proved in [6]. Biggs gave the equivalent result for effective resistances in [12].

Theorem 12 *Suppose that a block design has just two distinct concurrences, and that the pairs of vertices corresponding to the larger concurrence form the edges of a distance-regular graph H. Then pairwise variance increases with distance in H.*

7 Graph concepts linked to E-optimality

7.1 Measures of bottlenecks

A 'good' graph (for use as a network) is one without bottlenecks: any set of vertices should have many edges joining it to its complement. So, for any subset S of vertices, we let $\partial(S)$ (the *boundary* of S) be the set of edges which have one vertex in S and the other in its complement, and then define the *isoperimetric number* $\iota(G)$ by

$$\iota(G) = \min\left\{\frac{|\partial S|}{|S|} : S \subseteq V(G),\ 0 < |S| \leq \frac{v}{2}\right\}.$$

The next result shows that the isoperimetric number is related to the E-criterion. It is useful not so much for identifying the E-optimal designs as for easily showing that large classes of designs cannot be E-optimal: any design whose concurrence graph has low isoperimetric number performs poorly on the E-criterion.

Cutset Lemma 1 *Let G have an edge-cutset of size c whose removal separates the graph into parts S and $G \setminus S$ with m and n vertices respectively, where $0 < m \leq n$. Then*

$$\theta_1 \leq c\left(\frac{1}{m} + \frac{1}{n}\right) \leq \frac{2\,|\partial S|}{|S|}.$$

Proof We know that θ_1 is the minimum of $\mathbf{x}^\top \mathbf{L}\mathbf{x}/\mathbf{x}^\top \mathbf{x}$ over real vectors $\mathbf{x}$ with $\sum_i x_i = 0$. Put

$$x_i = \begin{cases} n & \text{if } i \in S \\ -m & \text{otherwise.} \end{cases}$$

Then $\mathbf{x}^\top \mathbf{x} = nm(m+n)$ and

$$\mathbf{x}^\top \mathbf{L}\mathbf{x} = \sum_{\text{edges } ij} (x_i - x_j)^2 = c(m+n)^2.$$

Hence

$$\theta_1 \leq \frac{\mathbf{x}^\top \mathbf{L}\mathbf{x}}{\mathbf{x}^\top \mathbf{x}} = \frac{c(m+n)^2}{nm(m+n)} = c\left(\frac{1}{m} + \frac{1}{n}\right) \leq \frac{2c}{m} = \frac{2\,|\partial S|}{|S|}. \quad \blacksquare$$

Corollary 1 *Let θ_1 be the smallest non-trivial eigenvalue of the Laplacian matrix $\mathbf{L}$ of the connected graph G. Then $\theta_1 \leq 2\iota(G)$.*

There is also an upper bound for the isoperimetric number in terms of θ_1, which is loosely referred to as a 'Cheeger-type inequality'; for details, see the further reading.

We also require a second cutset lemma, phrased in terms of vertex cutsets.

Cutset Lemma 2 *Let G have a vertex-cutset C of size c whose removal separates the graph into parts S and T with m, n vertices respectively (so $nm > 0$). Let m' and n' be the number of edges from vertices in C to vertices in S, T respectively. Then*

$$\theta_1 \leq \frac{m'n^2 + n'm^2}{nm(m+n)}.$$

In particular, if there are no multiple edges at any vertex of C then $\theta_1 \leq c$, with equality if and only if every vertex in C is joined to every vertex in $S \cup T$.

Proof Put

$$x_i = \begin{cases} n & \text{if } i \in S \\ -m & \text{if } i \in T \\ 0 & \text{otherwise.} \end{cases}$$

Then $\mathbf{x}^\top \mathbf{x} = nm(m+n)$ and $\mathbf{x}^\top \mathbf{L}\mathbf{x} = m'n^2 + n'm^2$, and so

$$\theta_1 \leq \frac{m'n^2 + n'm^2}{nm(m+n)}.$$

If there are no multiple edges at any vertex in C then $m' \leq cm$ and $n' \leq cn$ and the result follows. $\blacksquare$

7.2 Variance balance

A block design is *variance-balanced* if all the concurrences λ_{ij} are equal for $i \neq j$. In such a design, all of the pairwise variances V_{ij} are equal. Morgan and Srivastav proved the following result in [43].

Theorem 13 *If the constant concurrence λ of a variance-balanced design satisfies $(v-1)\lambda = \lfloor (bk/v) \rfloor (k-1)$ then the design is E-optimal.*

A block with k different treatments contributes $k(k-1)/2$ edges to the concurrence graph. Let us define the *defect* of a block to be

$$\frac{k(k-1)}{2} - \text{the number of edges it contributes to the graph.}$$

The following result is proved in [7].

Theorem 14 *If $k < v$, then a variance-balanced design with v treatments is E-optimal if the sum of the block defects is less than $v/2$.*

Table 1(b) shows that the design in Fig. 2(b) is variance-balanced. Block Γ_1 has defect 1, and each other block has defect 0, so the sum of the block defects is certainly less than 5/2, and Theorem 14 shows that the design is E-optimal. It is rather counter-intuitive that the non-binary design in Fig. 2(b) can be better than the design in Fig. 2(a); in fact, in his contribution to the discussion of Tocher's paper [51], which introduced this design, David Cox said

> I suspect that ... balanced ternary designs are of no practical value.

Computation shows that the design in Fig. 2(a) is Φ_p-better than the one in Fig. 2(b) if $p < 5.327$. In particular, it is A- and D-better.

8 Some history

As we have seen, if the experimental units form a single block and there are only two treatments then it is best for their replications to be as equal as possible. Statisticians know this so well that it is hard for us to imagine that more information may be obtained, about *all* treatment comparisons, if replications differ by more than 1.

In agriculture, or in any area with qualitative treatments, A-optimality is the natural criterion. If treatments are quantities of different substances,

then D-optimality is preferable, as the ranking on this criterion is invariant to change of measurement units. Thus industrial statisticians have tended to prefer D-optimality, although E-optimality has become popular among chemical process engineers. Perhaps the different camps have not talked to each other as much as they should have.

For most of the 20th century, it was normal practice in field experiments to have all treatments replicated three or four times. Where incomplete blocks were used, they typically had size from 3 to 20. Yates introduced his square lattice designs with $v = k^2$ in [55]. He used uniformity data and two worked examples to show that these designs can give lower average pairwise variance than a design using a highly replicated control treatment, but both of his examples were equireplicate with $r \in \{3, 4\}$.

In the 1930s, 1940s and 1950s, analysis of the data from an experiment involved inverting the Laplacian matrix without a computer: this is easy for BIBDs, and only slightly harder if the Laplacian matrix has only two distinct non-trivial eigenvalues. The results in [35] and [38] encouraged the beliefs that the optimal designs, on all Φ_p-criteria, are as equireplicate as possible, with concurrences as equal as possible, and that the same designs are optimal, or nearly so, on all of these criteria.

Three short papers in the same journal in 1977–1982 demonstrate the beliefs at that time. In [29], John and Mitchell did not even consider designs with unequal replication. They conjectured that, if there exist any regular-graph designs for given values of v, b and k, then the A- and D-optimal designs are regular-graph designs. For the parameter sets which they had examined by computer search, the same designs were optimal on the A- and D-criteria. In [33], Jones and Eccleston reported the results of various computer searches for A-optimal designs without the constraint of equal replication. For $k = 2$ and $b = v \in \{10, 11, 12\}$ (but not $v = 9$) their A-optimal design is almost a queen-bee design, and their designs are D-worse than those in [29]. The belief in equal replication was so ingrained that some readers assumed that there was an error in their program.

John and Williams followed this with the paper [30] on conjectures for optimal block designs for given values of v, b and k. Their conjectures included:

- the set of regular-graph designs always contains one that is optimal without this restriction;
- among regular-graph designs, the same designs are optimal on the A- and D-criteria.

They endorsed Cox's dismissal of non-binary designs, strengthening it to the

statement that they "are inefficient", and declared that the three unequally replicated A-optimal designs in [33] were "of academic rather than of practical interest". These conjectures and opinions seemed quite reasonable to people who had been finding good designs for the sizes needed in agricultural experiments.

At the end of the 20th century, there was an explosion in the number of experiments in genomics, using microarrays. Simplifying the story greatly, these are effectively block designs with $k = 2$, and biologists wanted A-optimal designs, but they did not know the vocabulary 'block' or 'A-optimal', 'graph' or 'cycle'. Computers were now much more powerful than in 1980, and researchers in genomics could simply undertake computer searches without the benefit of any statistical theory. In 2001, Kerr and Churchill [34] published the results of a computer search for A-optimal designs with $k = 2$ and $v = b \leq 11$. For $v \in \{10, 11, 12\}$, their results were completely consistent with those in [33], which they did not cite. They called cycles *loop designs*.

Mainstream statisticians began to get involved. In 2005, Wit, Nobile and Khanin published the paper [53] giving the results of a computer search for A- and D-optimal designs with $k = 2$ and $v = b$. The results are shown in Fig. 10. The A-optimal designs differ from the D-optimal designs when $v \geq 9$, but are consistent with those found in [34].

What is going on here? Why are the designs so different when $v \geq 9$? Why is there such a sudden, large change in the A-optimal designs? We explain this in the next section.

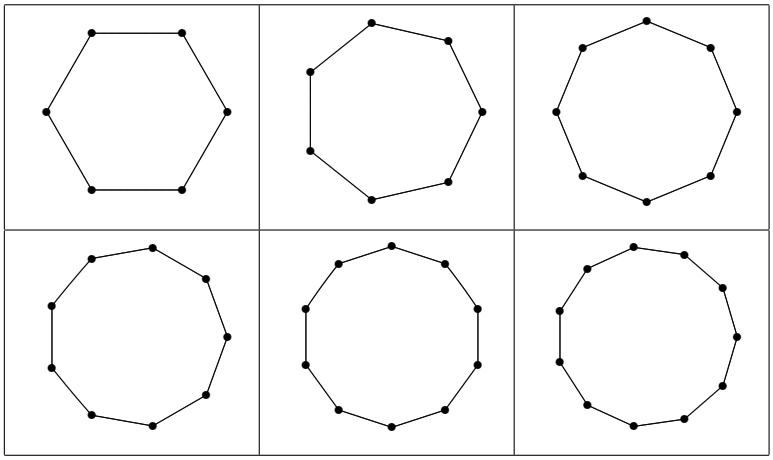
9 Block size two

9.1 Least replication

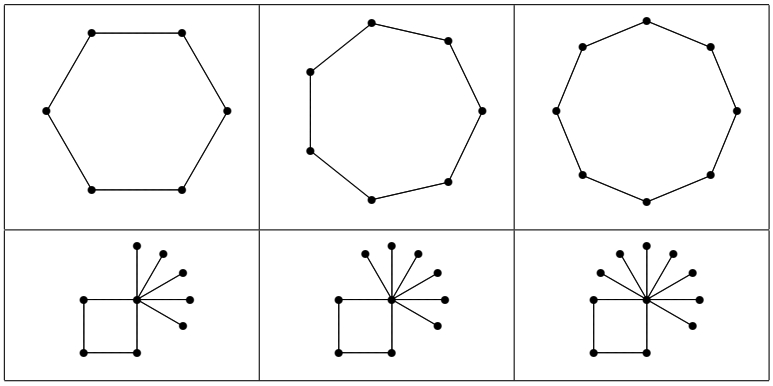
If $k = 2$, then the design is the same as its concurrence graph, and connectivity requires that $b \geq v - 1$. If $b = v - 1$, then all connected designs are trees, such as those in Fig. 11. Theorem 3 shows that the D-criterion does not differentiate between them.

In a tree, the effective resistance R_{ij} is just the length of the unique path between vertices i and j. Theorems 2 and 6 show that the only A-optimal designs are the stars, such as the graph on the right of Fig. 11.

In a star with v vertices, the contrast between any two leaves is an eigenvector of the Laplacian matrix $\mathbf{L}$ with eigenvalue 1, while the contrast between the central vertex and all the other vertices is an eigenvector with eigenvalue v. If $v \geq 5$ and G is not a star then there is an edge whose removal splits the graph into two components of sizes at least 2 and 3. Cut-



(a) D-optimal designs



(b) A-optimal designs

Figure 10: D-and A-optimal designs with $k = 2$ and $6 \leq v = b \leq 11$

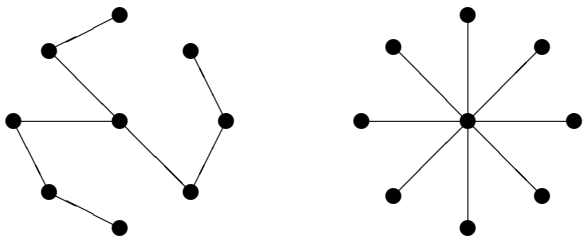


Figure 11: Two trees with $v = 9$, $b = 8$ and $k = 2$

set Lemma 1 then shows that $\theta_1 \leq 5/6 < 1$. The only other tree which is not a star is the path of length 3, for which direct calculation shows that $\theta_1 = 2 - \sqrt{2} < 1$. Hence the E-optimal designs are also the stars.

9.2 One fewer treatment

If $b = v$ and $k = 2$, then the concurrence graph G contains a single cycle: such graphs are called *unicyclic*. Let s be the length of the cycle. All the remaining vertices are in trees attached to various vertices of the cycle. Fig. 12 shows two unicyclic graphs with $v = 12$ and $s = 6$.

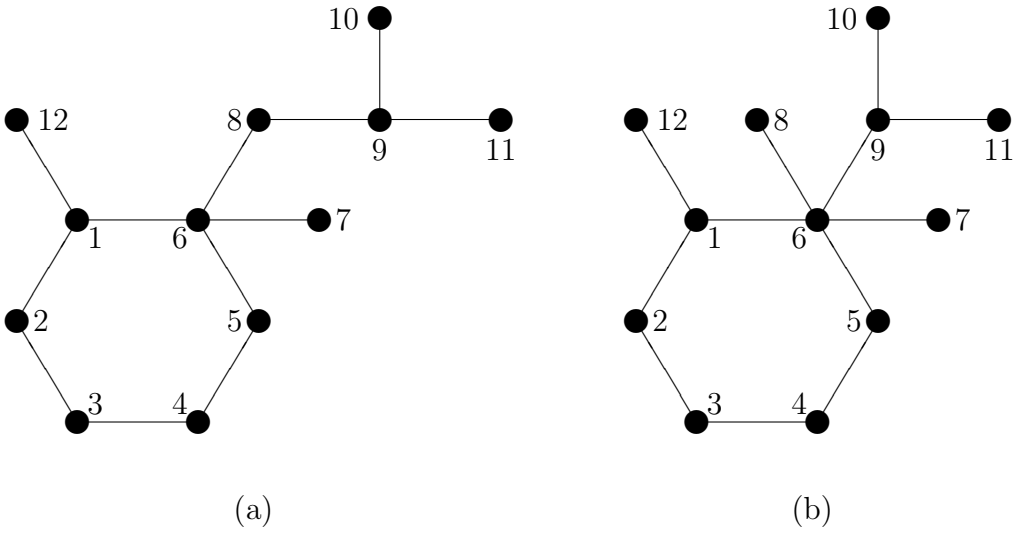


Figure 12: Two unicyclic graphs with $b = v = 12$ and $s = 6$

As we remarked in Section 5, the number of spanning trees in a unicyclic graph is equal to the length of the cycle. Hence, Theorem 3 gives the following result.

Theorem 15 *If $k = 2$ and $b = v \geq 3$, then the D-optimal designs are precisely the cycles.*

For A-optimality, we first show that no graph like the one in Fig. 12(a) can be optimal. If vertex 12 is moved so that it is joined to vertex 6, instead of vertex 1, then the sum of the variances $V_{i,12}$ for i in the cycle is unchanged and the variances $V_{i,12}$ for the remaining vertices i are all decreased. This argument shows that all the trees must be attached to the same vertex of the cycle.

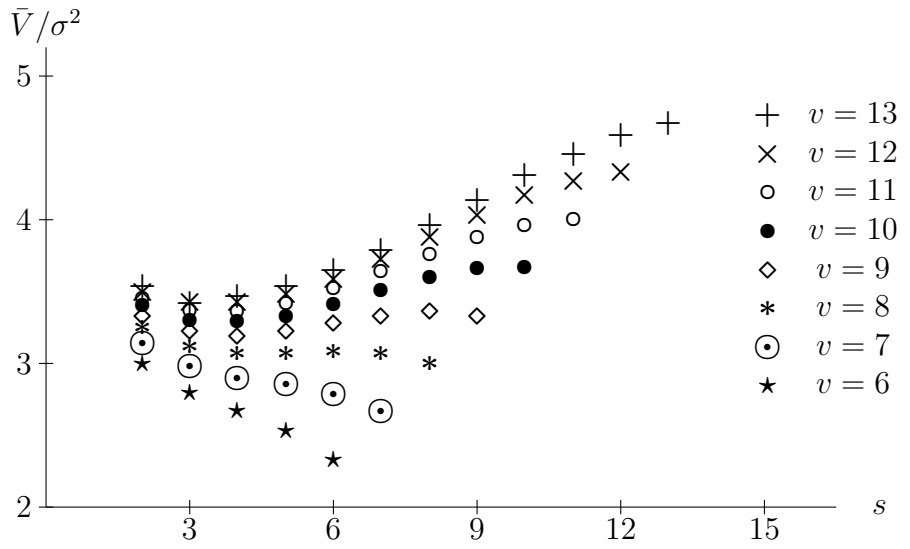


Figure 13: Average pairwise variance, in a unicylic graph with v vertices, as a function of the length s of the cycle

Now consider the tree on vertices 6, 8, 9, 10 and 11 in Fig. 12(a). If the two edges incident with vertex 8 are modified to those in Fig. 12(b), then the set of variances between these five vertices are unchanged, as are all others involving vertex 8, but those between vertices 9, 10, 11 and vertices outside this tree are all decreased. This argument shows that, for any given length s of the cycle, the only candidate for an A-optimal design has $v - s$ leaves attached to a single vertex of the cycle.

The effective resistance between a pair of vertices at distance d in a cycle of length s is $d(s-d)/s$, while that between a leaf and the cycle vertex to which it is attached is 1. Hence a short calculation shows that the sum of the pairwise effective resistances is equal to $g(s)/12$, where

$$g(s) = -s^3 + 2vs^2 + 13s - 12sv + 12v^2 - 14v.$$

Now $\bar{V}/\sigma^2 = g(s)/[3v(v-1)]$ and we seek the minimum of $g(s)$ for integers s in the interval $[2, v]$.

Fig. 13 plots $g(s)/[3v(v-1)]$ for s in $[2, v]$ and $6 \leq v \leq 13$. When $v \leq 7$, the function g is monotonic decreasing, so it attains its minimum on $[2, v]$ at $s = v$. For all larger values of v, the function g has a local minimum in the interval $[3, 5]$: when $v \geq 9$, the value at this local minimum is less than $g(v)$. This change from the upper end of the interval to the local minimum explains the sudden change in the A-optimal designs. Detailed examination of the local minimum gives the following result.

Theorem 16 *If $k = 2$ and $b = v \geq 3$ then the A-optimal designs are:*

- *a cycle, if $v \leq 8$;*
- *a square with $v - 4$ leaves attached to one vertex, if $9 \leq v \leq 11$;*
- *a triangle with $v - 4$ leaves attached to one vertex, if $v \geq 13$;*
- *either of the last two, if $v = 12$.*

What about E-optimality? The smallest eigenvalue of the Laplacian matrix of the triangle with one or more leaves attached to one vertex is 1, as is that of the digon with two or more leaves attached to one vertex. We now show that almost all other unicyclic graphs have at least one non-trivial eigenvalue smaller than this.

Suppose that vertex i in the cycle has a non-empty tree attached to it, so that $\{i\}$ is a vertex cutset. If $s \geq 3$ then there are no double edges, so Cutset Lemma 2 shows that $\theta_1 < 1$ unless all vertices are joined to i, in which case $s = 3$. If $s = 2$ and there are trees attached to both vertices of the digon, then applying Cutset Lemma 2 at each of these vertices shows that $\theta_1 < 1$ unless $v = 4$ and there is one leaf at each vertex of the digon: for this graph, $\theta_1 = 2 - \sqrt{5} < 1$. A digon with leaves attached to one vertex is just a star with one edge doubled.

The cycle of size v is a cyclic design. The smallest eigenvalue of its Laplacian matrix is $2(1 - \cos(2\pi/v))$, which is greater than 1 when $v \leq 5$, is equal to 1 when $v = 6$, and is less than 1 when $v \leq 7$. When $v = 3$ it is equal to 3, which is greater than $3 - \sqrt{3}$, which is the smallest Laplacian eigenvalue of the digon with one leaf.

Putting all of this together proves the following result.

Theorem 17 *If $k = 2$ and $b = v \geq 3$, then the E-optimal designs are:*

- *a cycle, if $v \leq 5$;*
- *a triangle with $v - 3$ leaves attached to one vertex, or a star with one edge doubled, if $v \geq 7$;*
- *either of the last two, if $v = 6$.*

Thus, for $v \geq 9$, the ranking on the D-criterion is essentially the opposite of the ranking on the A- and E-criteria. The A- and E-optimal designs are far from equireplicate. The change is sudden, not gradual. These findings were initially quite shocking to statisticians.

9.3 More blocks

What happens when b is larger than v but still has the same order of magnitude? The following theorems show that the A- and E-optimal designs are very different from the D-optimal designs when v is large. The proofs of Theorems 19 and 20 are in [4] and [7] respectively.

Theorem 18 *Let G be the concurrence graph of a connected block design Δ with $k = 2$ and $b \geq v$. If Δ is D-optimal then G does not contain any bridge (an edge cutset of size one): in particular, G contains no leaves.*

Proof Suppose that $\{i, j\}$ is an edge-cutset for G. Let H and K be the parts of G containing i and j, respectively.

Since G is not a tree, we may assume that H is not a tree, and so there is some edge e in H that is not in every spanning tree for H. Let n_1 and n_2 be the numbers of spanning trees for H that include and exclude e, respectively, and let m be the number of spanning trees for K. Every spanning tree for G consists of spanning trees for H and K together with the edge $\{i, j\}$. Hence G has $(n_1 + n_2)m$ spanning trees.

Let ℓ be a vertex on e with $\ell \neq i$. Form G' from G by removing edge e and inserting the edge e', where $e' = \{\ell, j\}$.

Let T and T' be spanning trees for H and K respectively. If T does not contain e then $T \cup \{\{i, j\}\} \cup T'$ and $T \cup \{e'\} \cup T'$ are both spanning trees for G'. If T contains e then $(T \setminus \{e\}) \cup \{\{i, j\}\} \cup \{e'\} \cup T'$ is a spanning tree for G'. Hence the number of spanning trees for G' is at least $(2n_2 + n_1)m$, which is greater than $(n_1 + n_2)m$ because $n_2 \geq 1$. Hence G does not have the maximal number of spanning trees and so Δ is not D-optimal. ∎

Theorem 19 *Let c be a positive integer. Then there is a positive integer v_c such that if $b - v = c$ and $v \geq v_c$ then all A-optimal designs with $k = 2$ contain leaves.*

Theorem 20 *If $20 \leq v \leq b \leq 5v/4$ then the concurrence graph for any E-optimal design with $k = 2$ contains leaves.*

Of course, to obtain a BIBD when $k = 2$, b needs to be a quadratic function of v. What happens if b is merely a linear function of v? In [7] we conjectured that if $b = cv$ for some constant c then there is a threshold result like the one in Theorem 19. However, current work by Robert Johnson and Mark Walters [32] suggests something much more interesting—that there is a constant C with $3 < C < 4$ such that if $b \geq Cv$ and $k = 2$ then all A-optimal designs are (nearly) equireplicate, and that random such graphs

(in a suitable model) are close to A-optimal with high probability. On the other hand if $b \leq Cv$ then a graph consisting of a large almost equireplicate part (all degrees 3 and 4 with average degree close to Cv) together with a suitable number of leaves joined to a single vertex is strictly better than any queen-bee design.

9.4 A little more history

The results on D- and A-optimality in Sections 9.1 and 9.2 were proved in [4], partly to put to rest mutterings that the results of [33, 34, 53] found by computer search were incorrect. The results on E-optimality are in [7].

In spite of the horror with which these results were greeted, it transpired that they were not new. The D- and E-optimal designs for $b = (v-1)/(k-1)$ were identified in [11] in 1991. The A-optimal designs for $k = 2$ and $b = v-1$ had been given in [41] in 1991. Also in 1991, Tjur gave the A-optimal designs for $k = 2$ and $b = v$ in [52]: his proof used the Levi graph as an electrical network.

A fairly common response to these unexpected results was 'It seems to be just block size 2 that is a problem.' Perhaps those of us who usually deal with larger blocks had simply not thought that it was worth while to investigate block size 2 before the introduction of microarrays.

However, as we sketch in the next section, the problem is not block size 2 but very low average replication. The proofs there are similar to those in this section; they are given in more detail in [8, 46]. Once again, it turns out that these results are not all new. The D-optimal designs for $v/(k-1)$ blocks of size k were given by Balasubramanian and Dey in [10] in 1996—but their proof uses a version of Theorem 5 with the wrong value of the constant. The A-optimal designs for $v/(k-1)$ blocks of size k were published by Krafft and Schaefer in [37] in 1997—but those authors are not blameless either, because they apparently had not read [52]!

Our best explanation is that agricultural statisticians are so familiar with average replication being at least 3 that when we saw these papers we decided that they had no applicability and so forgot them.

10 Very low average replication

In this section we once again consider general block size k. A block design is connected if and only if its Levi graph is connected. The Levi graph has $v + b$ vertices and bk edges, so connectivity implies that $bk \geq b + v - 1$; that is, $b(k-1) \geq v - 1$.

10.1 Least replication

If $b(k-1) = v-1$ and the design is connected, then the Levi graph $\tilde{G}$ is a tree and the concurrence graph G looks like those in Fig. 5. Hypergraph-theorists do not seem to have an agreed name for such designs.

For both D- and A-optimality, it turns out to be convenient to use the Levi graph. Since all the Levi graphs are trees, Theorem 5 shows that the D-criterion does not distinguish among connected designs.

By Theorem 7, $V_{ij} = \tilde{R}_{ij}\sigma^2$. When $\tilde{G}$ is a tree, $\tilde{R}_{ij} = 2$ when i and j are in the same block; otherwise, $\tilde{R}_{ij} = 4$ if any block containing i has a treatment in common with any block containing j; and otherwise, $\tilde{R}_{ij} \geq 6$. The queen-bee designs are the only ones for which $\tilde{R}_{ij} \leq 4$ for all i and j, and so they are the A-optimal designs.

The non-trivial eigenvalues of a queen-bee design are 1, k and v, with multiplicities $b-1$, $b(k-2)$ and 1, respectively. If the design is not a queen-bee design, then there is a treatment i that is in more than one block but not in all blocks. Thus vertex i forms a cutset for the concurrence graph G which is not joined to every other vertex of G. Cutset Lemma 2 shows that $\theta_1 < 1$. Hence the E-optimal designs are also the queen-bee designs.

10.2 One fewer treatment

If $b(k-1) = v$, then the Levi graph $\tilde{G}$ has bk edges and bk vertices, and so it contains a single cycle, which must be of some even length $2s$. If $2 \leq s \leq b$, then the design is binary; if $s = 1$, then there is a single non-binary block, whose defect is 1. In this case, $k \geq 3$, because each block must have more than one treatment.

For $2 \leq s \leq b$, let $\mathcal{C}(b, k, s)$ be the class of designs constructed as follows. Start with a loop design for s treatments. Insert $k-2$ extra treatments into each block. The remaining $b-s$ blocks all contain the same treatment from the loop design, together with $k-1$ extra treatments. Figs. 8 and 9 show the concurrence graph and Levi graph, respectively, of a design in $\mathcal{C}(6, 3, 6)$.

For $k \geq 4$, the designs in $\mathcal{C}(b, k, 1)$ have one treatment which occurs twice in one block and once in all other blocks, with the remaining treatments all replicated once. The class $\mathcal{C}(b, 3, 1)$ contains all such designs, and also those in which the treatment in every block is the one which occurs only once in the non-binary block.

Theorem 21 *If $b(k-1) = v$, then the D-optimal designs are those in $\mathcal{C}(b, k, b)$.*

Proof The Levi graph $\tilde{G}$ is unicyclic, so its number of spanning trees is maximized when the cycle has maximal length. Theorem 5 shows that the D-optimal designs are precisely those with $s = b$. ∎

Theorem 22 *If $b(k-1) = v$ then the A-optimal designs are those in $\mathcal{C}(b, k, s)$, where the value of s is given in Table 2.*

k \ b	2	3	4	5	6	7	8	9	10	11	12	13
2	2	3	4	5	6	7	8	4	4	4	3 or 4	3
3	2	3	4	5	6	3	3	3	3	3	2	2
4	2	3	4	5	3	2	2	2	2	2	2	2
5	2	3	4	5	2	2	2	2	2	2	2	2
6	2	3	4	2	2	2	2	2	2	2	2	2

Table 2: Value of s for A-optimal designs for $b(k-1)$ treatments in b blocks of size k: see Theorem 22

Proof The Levi graph $\tilde{G}$ has one cycle, whose length is $2s$, where $1 \leq s \leq b$. A similar argument to the one used at the start of the proof of Theorem 16 shows that this cannot be A-optimal unless the design is in $\mathcal{C}(b, k, s)$. If $s \geq 2$ or $k \geq 4$, then each block-vertex in the cycle has $k-2$ treatment-vertices attached as leaves; all other block-vertices are joined to the same single treatment-vertex in the cycle, and each has $k-1$ treatment vertices attached as leaves. In $\mathcal{C}(b, 3, 1)$ the first type of design has a Levi graph like this, and the other type has the same multiset of effective resistances between treatment-vertices, because their concurrence graphs are identical. The following calculations use the first type.

Let $\mathcal{V}_1$ be the set of treatment-vertices in the cycle, $\mathcal{V}_2$ the set of other treatment-vertices joined to blocks in the cycle, and $\mathcal{V}_3$ the set of remaining treatment-vertices. For $1 \leq i \leq j \leq 3$, denote by $\mathcal{R}_{ij}$ the sum of the pairwise resistances between vertices in $\mathcal{V}_i$ and $\mathcal{V}_j$.

Put

$$R_1 = \sum_{d=1}^{s-1} \frac{2d(2s-2d)}{2s} = \frac{s^2-1}{3}$$

and

$$R_2 = \sum_{d=0}^{s-1} \frac{(2d+1)(2s-2d-1)}{2s} = \frac{2s^2+1}{6}.$$

Then $\mathcal{R}_{11} = sR_1/2$, $\mathcal{R}_{12} = s(k-2)(R_2+s)$, $\mathcal{R}_{13} = (b-s)(k-1)(R_1+2s)$, $\mathcal{R}_{22} = s(k-2)(k-3) + s(k-2)^2[R_1 + 2(s-1)]/2$, $\mathcal{R}_{23} = (b-s)(k-1)(k-2)(R_2+3s)$, and $\mathcal{R}_{33} = (b-s)(k-1)(k-2)+2(b-s)(b-s-1)(k-1)^2$. Hence the sum of the pairwise effective resistances between treatment-vertices in the Levi graph is $g(s)/6$, where

$$g(s) = -(k-1)^2 s^3 + 2b(k-1)^2 s^2 - [6bk(k-1) - 4k^2 + 2k - 1]s + c$$

and $c = b(k-1)[12b(k-1) - 5k - 4]$.

If $s = 1$ then the design is non-binary. However,

$$g(1) - g(2) = (3k - 9 + 6b)(k-1) - 3,$$

which is positive, because $k \geq 2$ and $b \geq 2$. Therefore the non-binary designs are never A-optimal.

Direct calculation shows that $g(2) > g(3)$ when $b = 3$, and that $g(2) > g(3) > g(4)$ when $b = 4$. These inequalities hold for all values of k, even though g is not decreasing on the interval $[2, 4]$ for large k when $b = 4$.

If $b = 5$ and $k \geq 6$, then $g(3) > g(2)$ and $g(5) > g(2)$. Thus the local minimum of g occurs in the interval $(1, 3)$ and is the overall minimum of g on the interval $[1, 5]$.

Differentiation gives

$$g'(b) = b(k-1)[(b-6)(k-1) - 6] + 4k^2 - 2k + 1.$$

If $g'(b) > 0$ then g has a local minimum in the interval $(1, b)$. If, in addition, $g(3) > g(2)$, then the minimal value for integer s occurs at $s = 2$. These conditions are both satisfied if $k = 3$ and $b \geq 12$, $k = 4$ and $b \geq 8$, $k \geq 5$ and $b \geq 7$, or $k \geq 9$ and $b \geq 6$.

Given Theorem 16, there remain only a finite number of pairs (b, k) to be checked individually to find the smallest value of $g(s)$. The results are in Table 2. ∎

Theorem 23 *If $b(k-1) = v$, $b \geq 3$ and $k \geq 3$, then the E-optimal designs are those in $\mathcal{C}(b, k, b)$ if $b \leq 4$, and those in $\mathcal{C}(b, k, 2)$ and $\mathcal{C}(b, k, 1)$ if $b \geq 5$.*

Proof If $2 < s < b$ then the concurrence graph G has a vertex which forms a vertex-cutset and which is not joined to all other vertices; moreover, G has no multiple edges. Thus Cutset Lemma 2 shows that $\theta_1 < 1$.

Direct calculation shows that $\theta_1 = 1$ if $s = 1$ or $s = 2$. For $k \geq 4$, all contrasts between singly replicated treatments in the same block are eigenvectors of the Laplacian matrix L with eigenvalue k. When $k \geq 3$ and $s = b$

the contrast between singly and doubly replicated treatments has eigenvalue $2(k-1)$. For $s = b$, a straightforward calculation shows that the remaining eigenvalues of L are

$$k - \cos\left(\frac{2\pi n}{b}\right) \pm \sqrt{(k-1)^2 - \sin^2\left(\frac{2\pi n}{b}\right)}$$

for $1 \leq n \leq b-1$. The smallest of these is

$$k - \cos(2\pi/b) - \sqrt{(k-1^2) - \sin^2(2\pi/b)}\,:$$

this is greater than 1 if $b = 3$ or $b = 4$, but less than 1 if $k \geq 3$ and $b \geq 5$. ∎

11 Further reading

The Laplacian matrix of a graph, and its eigenvalues, are widely used, especially in connection with network properties such as connectivity, expansion, and random walks. A good introduction to this material can be found in the textbook by Bollobás [13], especially Chapters II (electrical networks) and IX (random walks). Connection between the smallest non-zero eigenvalue and connectivity is described in surveys by de Abreu [1] and by Mohar [42]. In this terminology, a version of Theorem 17 is in [24].

The basic properties of electrical networks can be found in textbooks of electrical engineering, for example Balabanian and Bickart [9]. A treatment connected to the multivariate Tutte polynomial appears in Sokal's survey [50]. Bollobás describes several approaches to the theory, including the fact (which we have not used) that the current flow minimises the power consumed in the network, and explains the interactions between electrical networks and random walks in the network. See also Deo [22].

The connection with optimal design theory was discussed in detail by the authors in their survey [7]. Further reading on optimal design can be found in John and Williams [31], Schwabe [47], or Shah and Sinha [48]. For general principles of experimental design, see Bailey [5].

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