



Optimal Incomplete-Block Designs with Low Replication: A Unified Approach Using Graphs

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Abstract

An incomplete-block design defines both a concurrence graph and a Levi graph. Properties of either graph can be used to compare designs with respect to D-optimality and with respect to A-optimality. In this paper, we show that optimality of the design implies strong conditions on connectivity properties of the graph, and use this to classify the optimal designs when the number of observational units is close to minimal.

Keywords Block design · A-optimality · D-optimality · Concurrence graph · Levi graph

Mathematics Subject Classification 62K05 · 62K10 · 05B05 · 05C40

1 Introduction

The purpose of this paper is to give a unified approach to the use of graph theory to find optimal incomplete-block designs with very low average replication. Some of the results given have already been proved by graph-theoretical or other methods.

The original online version of this article was revised: We regret the stylistic deficiencies in the earlier version. The current version represents the final version.

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Therefore a part of this paper gives historical notes on how graph theory has been used to determine optimal designs, while the other part continues this approach to give new results.

The two graphs associated with an incomplete-block design are its *Levi graph* and its *concurrency graph*. In [8], Bapat and Dey used the Levi graph to find D-optimal designs with the minimal number of observations, while Balasubramanian and Dey used it in [7] to find D-optimal designs with nearly minimal number of observations. In [33], Tjur used it to find A-optimal designs with nearly minimal number of observations when the block size is two, and Krafft and Schaefer extended this in [22] to arbitrary block size.

On the other hand, Cheng formulated D-optimality in terms of the concurrency graph in [11]. In [1], Bailey used this graph to find A-optimal and D-optimal designs when the block size is two and the average replication is low. Sajjad used it in [31] to find A- and D-optimal designs when the number of observations is minimal or nearly minimal.

Section 2 of this paper recalls definitions of block designs and related concepts, including the information matrix, the Laplacian matrix, D-optimality and A-optimality, and gives the notation used for the rest of the paper. The Levi graph and concurrency graph are defined, and examples are given.

Section 3 shows how the values of both optimality criteria can be determined from properties of either the concurrency graph or the Levi graph. Then Sect. 4 uses this to give some general results for D-optimal designs and A-optimal designs. Although the results are different for the two sorts of optimality, they both show that graphs associated with optimal designs have strong constraints on whether they can be disconnected by the removal of a single edge or a single vertex. Then Sects. 5 and 6 apply these results in a unified way to classify the optimal designs when the number of observational units is very low.

2 Definitions and Notation

2.1 Incomplete-Block Designs and Associated Matrices

Consider v treatments to be tested in b blocks of size k , where $2 \leq k < v$. Such a design is an *incomplete-block design*. A block design is said to be *connected* if all contrasts among treatment effects can be estimated, under the assumption that the expected value of each observation is the sum of an unknown fixed treatment effect and an unknown fixed block effect. The number of observations is bk , so a necessary condition for a block design to be connected is $bk \geq b + v - 1$. Put $c = bk - b - v + 1$. We need $c \geq 0$. Therefore $b(k - 1) \geq v - 1$, and so $b \geq (v - 1)/(k - 1) > 1$ because $k < v$.

Thus the number of observations is said to be *minimal* if $c = 0$ and *nearly minimal* if $c = 1$. The class of connected designs for given values of v , b , k and c is denoted $\mathcal{D}_c(v, b, k)$ in [7, 13]. The optimal designs with minimal or nearly minimal number of observations can be of special interest to a statistician. Two block designs in $\mathcal{D}_1(18, 6, 4)$ are shown in Fig. 1.

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

(a)
(b)

Fig. 1 Two block designs with $b = 6, k = 4$ and $v = 18$

We denote individual treatments by small Roman letters such as i and j , and individual blocks by large Greek letters such as Γ and Δ . Denote by $n_{i\Gamma}$ the number of times that treatment i occurs in block Γ . The design is said to be *binary* if $n_{i\Gamma} \leq 1$ for all i and Γ . Denote by r_i the number of observations on treatment i : thus

$$r_i = \sum_{\Gamma} n_{i\Gamma}.$$

Definition 1 The incidence matrix \mathbf{N} of an incomplete-block design is the $v \times b$ matrix whose (i, Γ) entry is $n_{i\Gamma}$.

Definition 2 Given an incomplete-block design, the *concurrence* λ_{ij} of treatments i and j is defined by

$$\lambda_{ij} = \sum_{\Gamma} n_{i\Gamma} n_{j\Gamma}.$$

If the design is binary, then $\lambda_{ii} = r_i$ and, for $i \neq j$, the concurrence λ_{ij} is the number of blocks in which i and j both occur. The concurrence matrix $\mathbf{\Lambda}$ is the $v \times v$ matrix with (i, j) entry equal to λ_{ij} . Therefore $\mathbf{\Lambda} = \mathbf{N}\mathbf{N}^T$.

Let \mathbf{R} be the $v \times v$ diagonal matrix with diagonal entries r_1, \dots, r_v , and denote by \mathbf{I}_b the identity matrix of order b . By standard linear model theory, the Fisher information matrix for estimating both treatment and block parameters is $\tilde{\mathbf{C}}$, where

$$\tilde{\mathbf{C}} = \begin{bmatrix} \mathbf{R} & \mathbf{N} \\ \mathbf{N}^T & k\mathbf{I}_b \end{bmatrix}.$$

The Fisher information matrix \mathbf{C} for the estimation of treatment effects only is given by $\mathbf{C} = \mathbf{R} - k^{-1}\mathbf{\Lambda}$. For all the treatment contrasts to be estimable, the rank of \mathbf{C} has to be $v - 1$. See [3,4,29,32,33].

2.2 Graphs Defined by Block Designs

We will discuss two graphs associated with block designs, the *Levi graph* and the *concurrence graph*. The Levi graph was introduced by Levi [24] and implicitly used by Bose in [9] in coining the concept of connectivity of a block design. In [12], Coxeter named it the *Levi graph*. Some authors call it the *incidence graph*. The concurrence graph was defined in [28] by Patterson and Williams as the *variety-concurrence graph*. It is worth mentioning here that Coxeter had called it the *Menger graph* in [12], and

that Grünbaum claimed in [17] that ‘The earlier ‘Menger graphs’ ... are much less useful.’

Definition 3 The *Levi graph* associated with an incomplete-block design is a bipartite graph with $v + b$ vertices. The vertices in one part are labelled by the treatments, those in the other part by the blocks. There are bk edges, one corresponding to each observation. An observation on treatment i in block Γ gives an edge between vertices i and Γ . Thus there are $n_{i\Gamma}$ edges between i and Γ , and bk edges in total. If the design is binary, then there is no more than one edge between any two vertices.

In any graph, the *degree* of a vertex denotes the number of edges incident with it. Thus in the Levi graph the degree $\text{deg}(\Gamma)$ of each block-vertex Γ is equal to k , while for each treatment-vertex $\text{deg}(i) = r_i$. The design can be recovered from its incidence matrix \mathbf{N} if its rows and columns are labelled and equivalently from its Levi graph if the vertices are labelled.

In a general graph with n vertices and e edges, the *cycle rank* is defined to be $e - n + 1$. This must be non-negative if the graph is connected. The Levi graph has $b+v$ vertices and bk edges, so c is equal to the cycle rank of the Levi graph. Henceforth, we shall call it the cycle rank of the block design.

Figures 2 and 3 show the Levi graphs of the block designs in Fig. 1a, b, respectively. Throughout this paper we use the convention that an open square represents a block-vertex and a filled circle represents a treatment-vertex.

Definition 4 The *concurrence graph* of an incomplete-block design is a graph whose vertices are labelled by the treatments. Distinct treatments i and j are joined by λ_{ij} edges.

In the concurrence graph, the degree of vertex i is given by $\text{deg}(i) = \sum_{\{j|j \neq i\}} \lambda_{ij}$. In general, two different block designs may have the same concurrence graphs: therefore

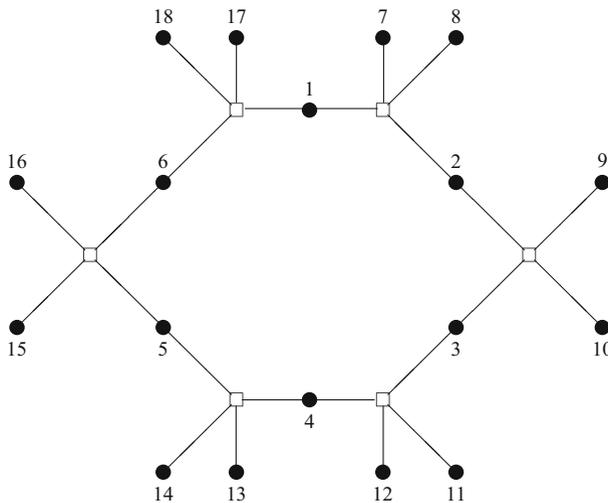


Fig. 2 Levi graph for the block design in Fig. 1a

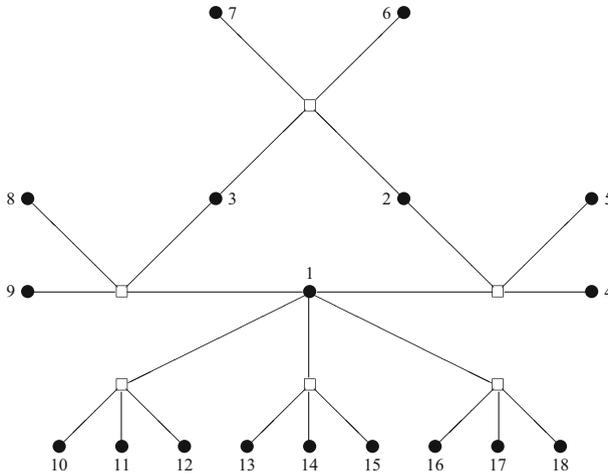


Fig. 3 Levi graph for the block design in Fig. 1b

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

(a)

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

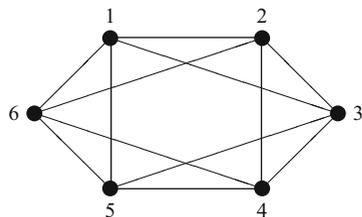
(b)

Fig. 4 Two block designs with $b = 4, k = 3$ and $v = 6$

the block design cannot be retrieved from its concurrence graph. For example, Fig. 4 shows two block designs with $v = 6, b = 4$ and $k = 3$ whose concurrence graph is the one shown in Fig. 5. In spite of this, the concurrence graph provides significant information to rank designs on different optimality criteria, as discussed by Bailey and Cameron in [3,4]. Furthermore, when $k = 2$, binary block designs are effectively the same as their concurrence graphs, with each edge corresponding to a block.

The following are equivalent: (i) an incomplete-block design is connected; (ii) its Levi graph is a connected graph; (iii) its concurrence graph is a connected graph. See [3,4,33].

Fig. 5 Concurrence graph for both designs in Fig. 4



2.3 Laplacian Matrices of Graphs

Definition 5 Let H be a graph on n vertices. The Laplacian matrix $\mathbf{L}(H)$ of this graph is the $n \times n$ matrix whose (i, j) entry L_{ij} is the negative of the number of edges between vertices i and j , if $i \neq j$, and whose (i, i) entry L_{ii} is the degree of i .

It follows from the above definition that $L_{ii} = -\sum_{\{j:j \neq i\}} L_{ij}$. Therefore the row and column sums of $\mathbf{L}(H)$ are all zero. Hence the Laplacian matrix $\mathbf{L}(H)$ has eigenvalue zero on the all-1 vector. Moreover, the multiplicity of this eigenvalue is equal to the number of connected components of H : see [3]. The other eigenvalues of $\mathbf{L}(H)$ are all positive. One way of proving this is to note that $\mathbf{L}(H)$ is the sum of matrices $\mathbf{L}_e(H)$ over all edges e of H , where the submatrix of $\mathbf{L}_e(H)$ corresponding to the two vertices joined by e is

$$\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

and all other entries of $\mathbf{L}_e(H)$ are zero: see [3]. It follows that $\mathbf{L}(H)$ is positive semi-definite.

Let G be the concurrence graph of a given incomplete-block design, and let \tilde{G} be its Levi graph. Let \mathbf{L} and $\tilde{\mathbf{L}}$ be the corresponding Laplacian matrices $\mathbf{L}(G)$ and $\mathbf{L}(\tilde{G})$. In [14–16], Gaffke showed that $\mathbf{L} = k\mathbf{C}$ and

$$\tilde{\mathbf{L}} = \begin{bmatrix} \mathbf{R} & -\mathbf{N} \\ -\mathbf{N}^T & k\mathbf{I}_b \end{bmatrix}.$$

It was shown in [4,33] that if the block parameters in the usual linear model are replaced by their negatives, then $\tilde{\mathbf{C}} = \tilde{\mathbf{L}}$.

We are interested only in connected incomplete-block designs whose blocks all have the same size. For such designs, zero has multiplicity one as an eigenvalue of \mathbf{C} and \mathbf{L} . The other eigenvalues of these matrices will be called *non-trivial*.

2.4 Optimality in Incomplete-Block Designs

These definitions are taken from [32].

Definition 6 An incomplete-block design for v treatments in b blocks of size k is called *D-optimal* if it maximizes the geometric mean of the non-trivial eigenvalues of the information matrix \mathbf{C} over all connected block designs for v treatments with b blocks of size k .

Equivalently, a D-optimal design minimizes the volume of the ellipsoid of confidence for the vector of treatment parameters. Equivalently again, a D-optimal design maximizes the geometric mean of the non-trivial eigenvalues of the Laplacian matrix \mathbf{L} .

Definition 7 An incomplete-block design is called *A-optimal* if it maximizes the harmonic mean of the non-trivial eigenvalues of the information matrix \mathbf{C} over all connected block designs for v treatments with b blocks of size k .

Equivalently, an A-optimal design minimizes the sum of the variances of the estimates of the differences between two treatment parameters. Equivalently again, an A-optimal design maximizes the harmonic mean of the non-trivial eigenvalues of the Laplacian matrix \mathbf{L} .

For both D- and A-optimality, the first equivalence is given in [29,32] and the second follows from the fact that $\mathbf{L} = k\mathbf{C}$.

3 Graphs and Optimality

3.1 Spanning Trees

Definition 8 A subset of the edges in a graph is a *cycle* if, together with the vertices at their ends, they form a connected subgraph in which every vertex has degree two. A subset of the edges (together with its vertices) is a *tree* if it is connected but contains no cycles. A tree whose vertices are all those of the original graph is a *spanning tree*.

Thus a connected graph is a tree if and only if $c = 0$, while, if $c = 1$, then it contains a single cycle.

Figure 6 shows a graph which is a tree: it has six vertices, five edges, and cycle rank zero. On the other hand, the Levi graph in Fig. 2 has a single cycle, which has length 12. Every spanning tree of this graph is made by removing a single edge of the cycle from the graph.

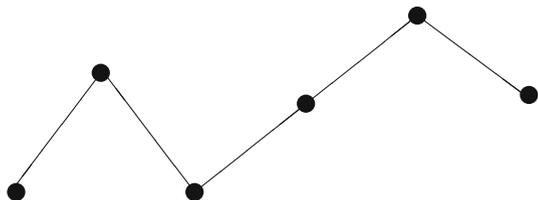
If a graph is not connected, it has no spanning trees. In [14], Gaffke showed the relevance to optimal design theory of the following theorem, known as the matrix tree theorem, which was given by Kirchhoff [21].

Theorem 1 If H is a connected graph with n vertices, then the product of n and the number of spanning trees of H is equal to the product of the non-trivial eigenvalues of $\mathbf{L}(H)$.

In [30], Sachs gave the next theorem, which was cited in [16].

Theorem 2 Let G and \tilde{G} be the concurrence graph and Levi graph, respectively, of an incomplete-block design for v treatments in b blocks of size k . Then the number of spanning trees of \tilde{G} is equal to the product of k^{b-v+1} and the number of spanning trees of G .

Fig. 6 A tree with six vertices and five edges



Since the product of the non-trivial eigenvalues of \mathbf{L} is their geometric mean raised to the power $v - 1$, these results give the following way of assessing D-optimality by using graphs.

Theorem 3 *Consider a connected incomplete-block design d for v treatments in b blocks of size k , with concurrence graph G and Levi graph \tilde{G} . The following statements are equivalent.*

- (i) *The design d is D-optimal.*
- (ii) *The graph G has the maximal number of spanning trees among concurrence graphs of such designs.*
- (iii) *The graph \tilde{G} has the maximal number of spanning trees among Levi graphs of such designs.*

Cheng used this theorem in [10,11] with the concurrence graph to find some D-optimal designs whose concurrence matrices are highly patterned. Gaffke used it in [16] with both graphs to find D-optimal designs for $v \leq 6$. Bapat and Dey used it in [8] with the Levi graph to show that all connected designs are D-optimal when $c = 0$. Balasubramanian and Dey extended this in [7] to find all D-optimal designs when $c = 1$ and $c = 2$, but unfortunately gave the wrong constant of proportionality in Sachs' theorem.

3.2 Electrical Networks

Denote by V_{ij} the variance of the best linear unbiased estimator of the difference between treatments i and j when the variance of each observation is unity. Thus

$$V_{ij} = C_{ii}^- + C_{jj}^- - 2C_{ij}^-,$$

where C_{ij}^- is the (i, j) entry of the Moore–Penrose generalized inverse \mathbf{C}^- of \mathbf{C} . Paterson and Wild used concurrence graphs to evaluate block designs in [26,27,35], using a heuristic argument that, in general terms, V_{ij} should increase according to the distance between vertices i and j in the graph G , where distance is the length of the shortest path connecting the two vertices. This is true for some nicely patterned graphs, but is not true in all cases, as shown in [2].

When microarray experiments became popular, there was a sudden need for A-optimal block designs with $k = 2$. The designs were drawn as their concurrence graphs. Jones and Eccleston [19], Kerr and Churchill [20] and Wit et al. [36] found A-optimal designs for small values of v and b by computer search. In [1], Bailey gave analytical proofs of these results, and extended them to larger values. In [3], Bailey and Cameron observed that V_{ij} is proportional, not to distance in G , but to *resistance-distance* in G , which is explained below. Tjur had already proved in [33] that V_{ij} is equal to resistance-distance in the Levi graph \tilde{G} , which he called the *design network*. He said “It is tempting to ask ... whether it makes sense to think of the variety-concurrence graph as an electrical network” and concluded that it does.

Any connected graph H can be considered as an electrical network with a 1-ohm resistance in each edge. Suppose that a battery is connected to vertices i and j , where

$i \neq j$, giving a potential difference of 1 volt between those vertices. Then current flows in the network according to the three standard laws of electrical networks.

Ohm's Law: In every edge, the (signed) current is equal to the (signed) potential difference between the vertices at its ends.

Kirchhoff's voltage law: The total (signed) potential difference around any cycle is zero.

Kirchhoff's current law: At every vertex except i and j , the total (signed) outgoing current is zero.

These laws give a unique solution for the total current between vertices i and j . The reciprocal of its absolute value is called the *effective resistance* or *resistance distance* between vertices i and j . Electrical network theory shows that this effective resistance is equal to $L_{ii}^- + L_{jj}^- - 2L_{ij}^-$, where L_{ij}^- is the (i, j) entry of the Moore–Penrose generalized inverse of $\mathbf{L}(H)$: see [6]. Thus results of [3,4,33,34] can be summarized as follows.

Theorem 4 *Let i and j be distinct treatments in an incomplete-block design with block size k . Let R_{ij} and \tilde{R}_{ij} be the effective resistances between i and j in the graphs G and \tilde{G} , respectively. Then $V_{ij} = \tilde{R}_{ij} = kR_{ij}$.*

This result gives an efficient method for calculating the values V_{ij} when the graph does not have many edges. Moreover, it gives the following analogue of Theorem 3.

Theorem 5 *Consider a connected incomplete-block design d for v treatments in b blocks of size k , with concurrence graph G and Levi graph \tilde{G} . The following statements are equivalent.*

- (i) *The design d is A-optimal.*
- (ii) *Among concurrence graphs of such designs, the graph G minimizes the sum of the resistance distances between pairs of distinct vertices.*
- (iii) *Among Levi graphs of such designs, the graph \tilde{G} minimizes the sum of the resistance distances between pairs of distinct treatment-vertices.*

For example, consider the resistance distance between treatment-vertices 1 and 3 in Fig. 2. The anticlockwise route around the cycle from 1 to 3 has eight edges, so, if a current of one amp goes on this route from vertex 1 to vertex 3, then the voltage difference between those two vertices is equal to eight volts. Then current will also flow along the shorter, clockwise route. This has four edges, and a voltage difference of eight volts, so the current must be two amps. Therefore the total current is three amps. The definition of effective resistance assumes a potential difference of 1 volt, so we scale so that the voltage difference is just one volt. This makes the current $3/8$, and so $\tilde{R}_{12} = 8/3$.

This example demonstrates the two key methods of combining resistance distances, which are explained in [6]. If two paths have a single vertex in common, then their union gives a single path: the resistance distance between its endpoints is the sum of the resistance distances of the original paths. This is known as combining resistances in series. If the two paths have the same endpoints but no other vertices in common, then their resistance distances are in parallel: to combine these, we add the reciprocals of both, and then invert that.

3.3 Which Graph to Use?

When $k = 2$, the concurrence graph is effectively the same as the design, and it seems natural to use it to calculate the number of spanning trees and the pairwise effective resistances. When $k = 3$, both graphs have $3b$ edges, but the Levi graph has more vertices, so again it is simpler to use the concurrence graph. For larger values of k , the Levi graph has fewer edges, and the concurrence graph has b complete subgraphs of size k , so that calculations become simpler in the Levi graph. For theorems valid for all values of k , it seems simpler to use the Levi graph, although visualizing the graph for a given design with small k is easier with the concurrence graph. If $b > v - 1$, then Theorem 2 shows that the Levi graph has more spanning trees and so it may be easier to count them in the concurrence graph; if $b < v - 1$, then it is the other way around.

The remaining sections of the paper prove some general results valid for all values of k , so the proofs are given using the Levi graph in all cases.

4 Bridges and Cut-Vertices

4.1 Definitions

One way of measuring the connectivity of a graph is to find out how many edges (or vertices) need to be removed to disconnect the graph.

Definition 9 An edge of a connected graph is a *bridge* if its removal disconnects the graph. A vertex of a connected graph is a *cut-vertex* if its removal (together with all edges incident to it) leaves a disconnected graph.

Thus, if a graph is a tree, then every edge is a bridge.

For example, in Fig. 3, vertex 1 is a cut-vertex. The three edges coming down from that vertex are all bridges. Vertex 4 is not a cut-vertex, but the single edge incident with that vertex is a bridge.

A bridge in the Levi graph corresponds to an observation whose loss makes some treatment contrast inestimable. In the terminology of Latif et al. [23], if the Levi graph has a bridge, then the design has *breakdown number* one.

Lemma 1 Suppose that a connected graph K has a cut-vertex W , cutting it into components H_1 and H_2 both containing W . Let c , c_1 and c_2 be the cycle ranks of K , H_1 and H_2 , respectively. Then $c = c_1 + c_2$.

Proof For $m = 1, 2$, suppose that H_m contains e_m edges and v_m vertices in addition to W . See Fig. 7. Then $c_m = e_m - v_m$ for $m = 1, 2$. The graph K has $e_1 + e_2$ edges and $v_1 + v_2 + 1$ vertices, and so $c = e_1 + e_2 - v_1 - v_2 = c_1 + c_2$. \square

In the rest of this section, we show that optimality places strong conditions on the potential occurrences of bridges and cut-vertices in the Levi graph.

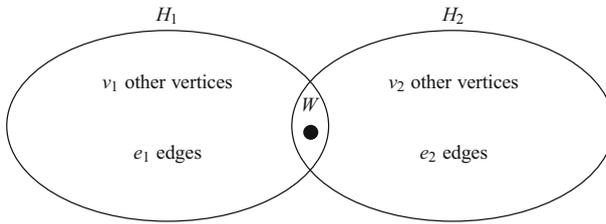


Fig. 7 Graph in the proof of Lemma 1: W is a cut-vertex

4.2 General Results for D-optimality

In [5], Bailey, Schiffl and Hilgers proved the following.

Theorem 6 *If G is the concurrence graph of a D-optimal block design with $k = 2$, $v \geq 3$ and $c \geq 1$, then G does not contain a bridge.*

When $k = 2$, the Levi graph has a bridge if and only if the concurrence graph has a bridge, so Theorem 6 can be rephrased in terms of the Levi graph. Here we prove a stronger result.

Theorem 7 *Let \tilde{G} be the Levi graph of a D-optimal block design d with $c \geq 1$. Then \tilde{G} does not contain any bridge, except, possibly, a bridge whose treatment-vertex has degree 1.*

Proof Since $c \geq 1$, \tilde{G} is not a tree, so, if it does contain a bridge, then it contains a bridge e joining treatment-vertex i to block-vertex Γ in which at least one of those two vertices is contained in a cycle of \tilde{G} . If e is removed, then \tilde{G} splits into two connected components. Denote by H and K the components containing i and Γ , respectively. There are no other edges between H and K .

First, suppose that i is contained in a cycle in H , and that f is one edge of this cycle, joining treatment-vertex i to block-vertex Δ . See Fig. 8. Let n_1 be the number of spanning trees of H which contain f , and let n_2 be the number of spanning trees of H which do not contain f . Because f is in a cycle, $n_2 > 0$. Let m be the number of spanning trees of K . The block-vertex Γ has degree k , so it has $k - 1$ edges in K , so K has more than one vertex. Therefore, because K is connected, $m > 0$. Every spanning tree of \tilde{G} consists of a spanning tree for H , the bridge e , and a spanning tree for K . Therefore \tilde{G} has $(n_1 + n_2)m$ spanning trees, where $n_2 > 0$.

Let j be one of the treatment-vertices in K which are joined to block-vertex Γ . Create a new design d^* from d by removing i from Δ and replacing it by j , so that all blocks still have size k . Let \tilde{G}^* be the Levi graph of d^* , which omits the edge f but contains the edge e' between j and Δ . Let T and T' be spanning trees for H and K respectively. If T does not contain f , then $T \cup \{e\} \cup T'$ and $T \cup \{e'\} \cup T'$ are both spanning trees for \tilde{G}^* ; if T does contain f , then $(T \setminus \{f\}) \cup \{e, e'\} \cup T'$ is a spanning tree for \tilde{G}^* . Therefore the number of spanning trees for \tilde{G}^* is at least $(n_1 + 2n_2)m$, which is strictly greater than $(n_1 + n_2)m$ because $n_2 > 0$ and $m > 0$. This contradicts the D-optimality of design d .

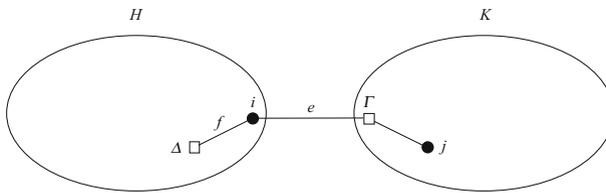


Fig. 8 Graph in the first case in the proof of Theorem 7: e is a bridge

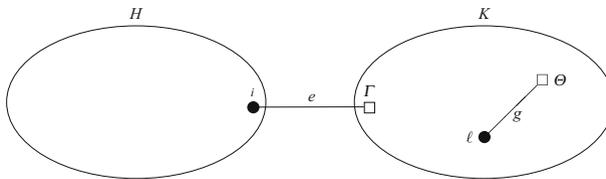


Fig. 9 Graph in the second case in the proof of Theorem 7: e is a bridge

Secondly, suppose that Γ is contained in a cycle in K . The argument is similar, but with some modifications, so we give it in full. Let g be one edge in this cycle, joining treatment-vertex ℓ to block-vertex Θ (which may or may not be the same as Γ). See Fig. 9. Let m_1 be the number of spanning trees of K which contain g , and let m_2 be the number of spanning trees of K which do not contain g . Then $m_2 > 0$. Let n be the number of spanning trees of H . If $\deg(i) > 1$, then H has more than one vertex and so $n > 0$; if $\deg(i) = 1$, then H consists of the single vertex i , which by itself forms the only spanning tree for H , and so $n = 1$. In both cases, the number of spanning trees of \tilde{G} is $(m_1 + m_2)n$.

Create a new design d^{**} from d by removing ℓ from Θ and replacing it by i ; all blocks still have size k . The Levi graph \tilde{G}^{**} of d^{**} is obtained from \tilde{G} by removing the edge g and inserting an edge e'' between i and Θ . Let T and T' be spanning trees for H and K respectively. If T' does not contain g , then $T \cup \{e\} \cup T'$ and $T \cup \{e''\} \cup T'$ are both spanning trees for \tilde{G}^{**} ; if T' does contain g , then $T \cup \{e, e''\} \cup (T' \setminus \{g\})$ is a spanning tree for \tilde{G}^{**} . Therefore the number of spanning trees for \tilde{G}^{**} is at least $(m_1 + 2m_2)n$, which is strictly greater than $(m_1 + m_2)n$ as $m_2 > 0$ and $n > 0$, again contradicting the D-optimality of design d . \square

As an example of the proof of Theorem 7, consider the block design in Fig. 1b. Its Levi graph is in Fig. 3. This has a single cycle, which has length 6, so it has 6 spanning trees. Let e be the bridge joining treatment-vertex 1 to the vertex for the block Γ containing treatment 18, and let f be the edge joining treatment-vertex 1 to the block Δ containing treatment 2. Create the new design by removing treatment 1 from Δ and replacing it by treatment 18. The new design has a single cycle of length 8, containing the vertices for treatments 2, 3, 1 and 18 in order, so it has 8 spanning trees.

Note that, if $bk < 2v$, then the design must have at least one treatment i with $r_i = 1$ and so even a D-optimal design will have a bridge in which one of its vertices has degree 1. A vertex with degree 1 is called a *leaf*. Let us call a bridge *leafless* if neither of its vertices is a leaf.

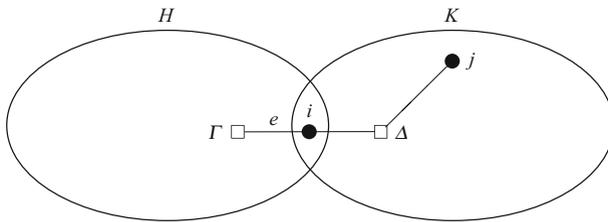


Fig. 10 Graph in the proof of Theorem 8: i is a cut-vertex

Theorem 8 *If \tilde{G} is the Levi graph of a D -optimal block design d with $c \geq 1$, then no treatment-vertex of \tilde{G} is a cut-vertex.*

Proof Suppose that treatment-vertex i is a cut-vertex which splits \tilde{G} into components H and K both containing i as well as other vertices. Thus $\deg(i) \geq 2$ and there are no edges between H and K except those through vertex i . Let e be an edge through i in H , joining i to block-vertex Γ . Since $c \geq 1$, Theorem 7 shows that e is not a bridge. Therefore e is contained in a cycle in H . Hence there is at least one spanning tree for H which contains e , and at least one which omits it. See Fig. 10.

Suppose that i is joined to block-vertex Δ in K . Because $\deg(\Delta) \geq 2$, there is a treatment-vertex j joined to Δ with $j \neq i$. Create a new design d^* from d by removing i from Γ and replacing it by j . The Levi graph \tilde{G}^* of d^* is obtained from \tilde{G} by replacing the edge e with an edge f connecting j to Γ .

Every spanning tree of \tilde{G} has the form $T \cup T'$, where T and T' are spanning trees for H and K respectively. Thus the number of spanning trees for \tilde{G} is $n_1 n_2$, where n_1 and n_2 are the number of spanning trees for H and K respectively. If T contains e , then $(T \setminus \{e\}) \cup \{f\} \cup T'$ is a spanning tree for \tilde{G}^* . If T does not contain e , then $T \cup T'$ is a spanning tree for \tilde{G}^* . Furthermore, T' contains a unique path from i to j , and this has positive even length (it may not be the path through vertex Δ shown in Fig. 10, because T' does not contain all edges in K). If e' is any one of the edges in this path, then $T \cup \{f\} \cup (T' \setminus \{e'\})$ is a spanning tree for \tilde{G}^* . Different choices for T' may give rise to the same spanning tree of this type. Nevertheless, at least two of them are distinct, and so the number of spanning trees for \tilde{G}^* is at least $n_1 n_2 + 2$, which contradicts the D -optimality of d . □

4.3 General Results for A-optimality

Theorem 9 *Suppose that i is a treatment in a block design d and that its treatment-vertex is a cut-vertex of the Levi graph \tilde{G} of d , cutting it into components H_1 and H_2 both containing i . For $m = 1, 2$, let H_m contain v_m treatment-vertices in addition to i , let R_m be the sum of the resistance distances between pairs of treatment-vertices in H_m and let S_m be the sum of these in H_m which involve treatment-vertex i . Let K_m be the set of treatment-vertices, including i , in H_m . Thus $S_m = \sum_{j \in K_m} \tilde{R}_{ij}$, because $\tilde{R}_{ii} = 0$, and $R_m = (\sum_{j \in K_m} \sum_{\ell \in K_m} R_{j\ell})/2$, because $\tilde{R}_{jj} = 0$ and $\tilde{R}_{j\ell} = \tilde{R}_{\ell j}$ for all*

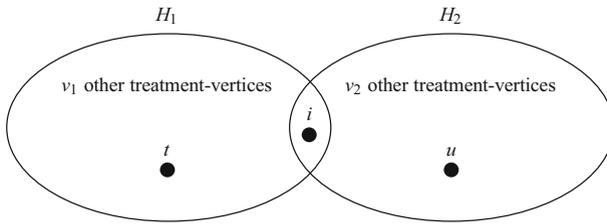


Fig. 11 Graph in the proof of Theorem 9: i is a cut-vertex

j and l . Then the sum of the resistance distances between pairs of treatment-vertices in \tilde{G} is $R_1 + R_2 + v_2S_1 + v_1S_2$.

Proof See Fig. 11. All resistance distances involving treatment-vertex i within H_1 or H_2 are included in $R_1 + R_2$. If t is a treatment-vertex in $K_1 \setminus \{i\}$ and u is a treatment-vertex in $K_2 \setminus \{i\}$, then $\tilde{R}_{tu} = \tilde{R}_{ti} + \tilde{R}_{iu}$. Summing this over all t and u gives $v_2S_1 + v_1S_2$, and the result follows. \square

The following lemma shows the use of Theorem 9 on a small example. Not only does this help in understanding Theorem 9; it will also be used in the proof of Theorem 11.

Lemma 2 *In addition to the assumptions and notation in Theorem 9, suppose that $k = 3$ and $v_1 = 4$. Suppose that component H_1 is as shown in Fig. 12a, so that block Δ contains treatments i, t and u , while block Γ contains treatment j twice and treatment i once. Then d is not A-optimal.*

Proof In H_1 , the resistance distances between pairs of treatment-vertices are

$$\tilde{R}_{ij} = 3/2, \tilde{R}_{it} = \tilde{R}_{iu} = \tilde{R}_{tu} = 2 \text{ and } \tilde{R}_{jt} = \tilde{R}_{ju} = 7/2.$$

Hence $R_1 = 29/2$ and $S_1 = 11/2$.

Construct a new design d^* from d by removing one occurrence of j from Γ , inserting it into Δ , and removing t from Δ and inserting it into Γ , thus giving H_1^* in Fig. 12b. The resistance distances between pairs of treatment-vertices in H_1^* are

$$\tilde{R}_{ij}^* = 1, \tilde{R}_{it}^* = \tilde{R}_{iu}^* = \tilde{R}_{jt}^* = \tilde{R}_{ju}^* = 7/4 \text{ and } \tilde{R}_{tu}^* = 3.$$

Hence $R_1^* = 11 < R_1$ and $S_1^* = 9/2 < S_1$.

Theorem 9 shows that the sum of the resistance distances between pairs of treatment-vertices in the Levi graph is

$$\begin{aligned} R_1 + R_2 + v_2S_1 + 4S_2 & \text{ for design } d, \text{ and} \\ R_1^* + R_2 + v_2S_1^* + 4S_2 & \text{ for design } d^*. \end{aligned}$$

Since $R_1^* < R_1$ and $S_1^* < S_1$, the second value is strictly smaller, regardless of the properties of H_2 . By Theorem 5, the design d cannot be A-optimal. \square

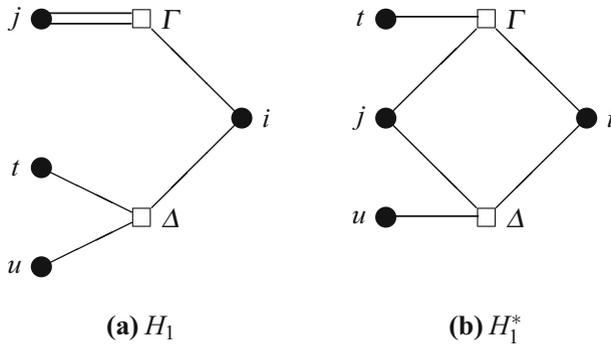


Fig. 12 Two possibilities for one component of the Levi graph in Lemma 2

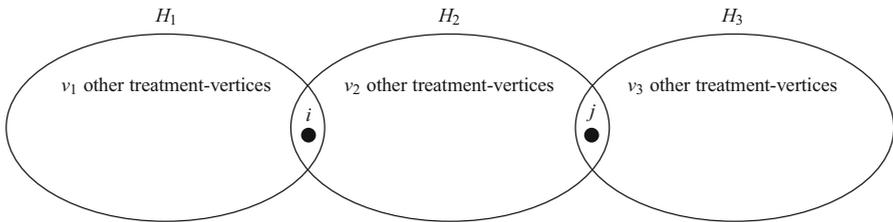


Fig. 13 Graph in the proof of Theorem 10: i and j are both cut-vertices

Theorem 10 Let \tilde{G} be the Levi graph of an A -optimal block design d . Then there cannot be two distinct treatments i and j whose vertices are both cut-vertices.

Proof Suppose that there are two such treatments i and j . Then removing vertices i and j splits the graph \tilde{G} into three components H_1 , H_2 and H_3 , each with at least two vertices, where treatment-vertex i is the only vertex in $H_1 \cap H_2$, treatment-vertex j is the only vertex in $H_2 \cap H_3$ and $H_1 \cap H_3$ contains no vertices. Each component must be connected, because the whole Levi graph is connected. For $\ell \in \{1, 2, 3\}$, let K_ℓ be the set of treatment-vertices in H_ℓ , and let $v_\ell = |K_\ell \setminus \{i, j\}|$. See Fig. 13.

Let

$$S_1 = \sum_{t \in K_1} \tilde{R}_{it}, \quad S_2 = \sum_{t \in K_2} \tilde{R}_{it}, \quad S_3 = \sum_{t \in K_2} \tilde{R}_{jt} \quad \text{and} \quad S_4 = \sum_{t \in K_3} \tilde{R}_{jt}.$$

Then

$$\sum_{t \in K_1} \tilde{R}_{jt} = S_1 + (v_1 + 1)\tilde{R}_{ij} \quad \text{and so} \quad \sum_{t \in K_1 \cup K_2} \tilde{R}_{jt} = S_3 + S_1 + v_1\tilde{R}_{ij}$$

(after removing the double occurrence of \tilde{R}_{ij} , because $K_1 \cap K_2 = \{i\}$).

Let R_0 and R_3 be the sums of the resistance distances between pairs of treatment-vertices in $K_1 \cup K_2$ and K_3 , respectively. Theorem 9 shows that the sum of the resistance distances between pairs of treatment-vertices in \tilde{G} is

$$R_0 + R_3 + (v_1 + v_2 + 1)S_4 + v_3(S_1 + S_3 + v_1\tilde{R}_{ij}). \tag{1}$$

There is no loss of generality in assuming that $S_2 \leq S_3$. Create design d^* from d by replacing treatment j by treatment i in all those blocks containing j whose other treatment-vertices are in K_3 . Let \tilde{G}^* be the Levi graph of d^* , and denote resistance distances in this graph by \tilde{R}^* . Then

$$\sum_{t \in K_1 \cup K_2} \tilde{R}_{it}^* = S_1 + S_2,$$

and so Theorem 9 shows that the sum of the resistance distances between pairs of treatment-vertices in \tilde{G}^* is

$$R_0 + R_3 + (v_1 + v_2 + 1)S_4 + v_3(S_1 + S_2). \tag{2}$$

Since $S_2 \leq S_3$ and $0 < v_1v_3\tilde{R}_{ij}$, the comparison of expressions (1) and (2) shows that the sum of the resistance distances between pairs of treatment-vertices in \tilde{G}^* is strictly less than the corresponding sum in \tilde{G} , which contradicts the A-optimality of d , by Theorem 5. \square

Theorem 11 *If \tilde{G} is the Levi graph of an A-optimal block design d with $c \geq 1$, then no treatment-vertex of \tilde{G} is a cut-vertex unless it is contained in a cycle.*

Proof Suppose that treatment i gives such a cut-vertex, contained in no cycle and cutting \tilde{G} into components H_1 and H_2 both containing i . Without loss of generality, there is a cycle in H_1 . If $H_1 \setminus \{i\}$ is not connected then we may move any, but not all, of its connected components into H_2 without affecting the assumptions, so long as we leave a cycle in H_1 . Thus we may assume that $H_1 \setminus \{i\}$ is connected.

Suppose that treatment i is in blocks Γ_1 and Γ_2 whose vertices are in H_1 . Since $H_1 \setminus \{i\}$ is connected, it contains a path from Γ_1 to Γ_2 . Adding the edges from Γ_1 and Γ_2 to i gives a cycle containing vertex i . This is contradicts our assumption that i is not in a cycle.

Otherwise, suppose that treatment i is in a unique block Γ in H_1 . Because H_1 is connected and contains a cycle, there is at least one treatment-vertex j in H_1 that is joined to Γ and is not a leaf. See Fig. 14. If the edge between Γ and j is not in a cycle, then j is also a cut-vertex, which contradicts Theorem 10. Hence this edge is in a cycle. If the cycle has length $2n$, then the rule for combining resistance distances in parallel given in Sect. 3.2 shows that

$$\tilde{R}_{j\Gamma} \leq \left[1 + \frac{1}{2n - 1} \right]^{-1} = \frac{2n - 1}{2n} < 1.$$

On the other hand, $\tilde{R}_{i\Gamma} = 1$ because the edge between Γ and i is not contained in any cycle. In particular, there cannot be multiple edges between Γ and i .

For $m = 1, 2$, let R_m be the sum of the resistance distances between pairs of treatment-vertices in H_m , and let v_m be the number of treatment-vertices in H_m in

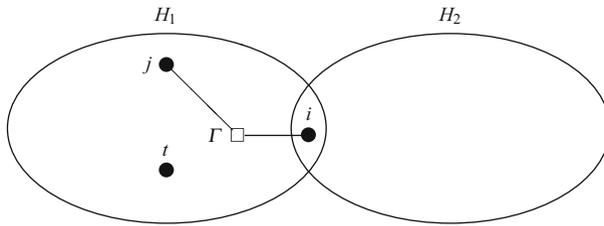


Fig. 14 Graph in the proof of Theorem 11: j is a cut-vertex not contained in a cycle

addition to i . Let S_i and S_j be the sum of resistance distances between treatment-vertices in H_1 and vertices i and j , respectively, and let S be the sum of resistance distances between vertex i and treatment-vertices in H_2 . Theorem 9 shows that the sum of the resistance distances for pairs of treatment-vertices in \tilde{G} is $R_1 + R_2 + v_2 S_i + v_1 S$.

Let t be a treatment, other than i and j , whose vertex is in H_1 . Because resistance distance is a metric,

$$\tilde{R}_{jt} \leq \tilde{R}_{j\Gamma} + \tilde{R}_{\Gamma t} < 1 + \tilde{R}_{\Gamma t} = \tilde{R}_{it}.$$

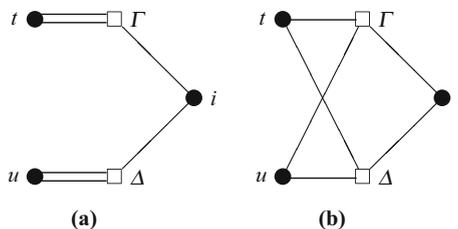
Hence $S_j < S_i$.

Create a new design d^* from d by replacing treatment i with treatment j in every block containing i whose vertex is in H_2 . Then the sum of the resistance distances for pairs of treatment-vertices in the new Levi graph is $R_1 + R_2 + v_2 S_j + v_1 S$, which is strictly less than it was in \tilde{G} . This contradicts the A-optimality of d , by Theorem 5.

The last step in the proof breaks down if i and j are the only treatment-vertices in H_1 . In this case, j is joined to Γ by at least two edges. As noted above, there is only one edge between i and Γ . Hence there are $k - 1$ edges between j and Γ . Thus $\tilde{R}_{ij} = 1 + 1/(k - 1) = k/(k - 1)$. If $k \geq 4$, then replacing one occurrence of treatment j in block Γ by a second copy of treatment i reduces \tilde{R}_{ij} to $1/2 + 1/(k - 2) = k/(2k - 4)$. This reduces all the resistance distances from j to treatment-vertices within H_2 , while leaving all those within H_2 unchanged. Thus d cannot be A-optimal, by Theorem 5.

The only remaining possibility is that $k = 3$ and that vertex i cuts \tilde{G} into connected components, each containing one block. At least one block contains two copies of one treatment, which is not i . The remaining blocks are either like this or contain three distinct treatments. Hence there are either a pair of components giving the graph in Fig. 12a or there are a pair giving the graph in Fig. 15a. In the first case, Lemma 2

Fig. 15 Two possibilities for one component of the Levi graph at the end of the proof of Theorem 11



shows that d is not A-optimal. In the second case, a similar argument shows that replacing the graph in Fig. 15a by the one in Fig. 15b, while leaving the rest of the design unchanged, gives a design with a strictly smaller sum of resistance distances between pairs of treatment-vertices, and so d is not A-optimal, by Theorem 5. \square

5 D-optimal Block Designs with Low Cycle Rank

5.1 Minimal Number of Observations

Theorem 12 *If $bk = b + v - 1$, then all connected block designs for v treatments in b blocks of size k are D-optimal.*

Proof In this case, the number of edges of the Levi graph is one less than its number of vertices. Hence, if it is connected, then it must be a tree, and so it has precisely one spanning tree. If it is not connected, it has none. \square

Theorem 12 was proved in [8,25]. We include it here for completeness.

5.2 Nearly Minimal Number of Observations

Since $c = bk - b - v + 1$, $c = 1$ if and only if $v = b(k - 1)$. Thus there is a single cycle if and only if $v = b(k - 1)$. In this case, $b = v/(k - 1) \leq v$ and so $\min\{b, v\} = b$.

Theorem 13 *If $bk = b + v$, then every D-optimal design is obtainable from the following by relabelling treatments and relabelling blocks. For $i = 1, \dots, b - 1$, block Γ_i contains treatments i and $i + 1$, while block Γ_b contains treatments b and 1. A further $k - 2$ treatments, all with replication 1, are inserted into each block.*

Proof In this case, the Levi graph contains a single cycle. Each spanning tree is obtained by removing one edge from the cycle, so the design is D-optimal if and only if the cycle has maximal length, which is $\min\{v, b\} = b$. \square

For example, this theorem shows that the block design in Fig. 1a is D-optimal.

Theorem 13 was proved in [7]. Again, we include it both for completeness and to show the benefit of the unified approach.

5.3 One More Observation

If $bk = b + v + 1$, then $c = 2$. Let \tilde{G} be the Levi graph of a block design d for v treatments in b blocks of size k . When $c = 2$, then there are only three possibilities for how the cycles occur in a graph: (a) there are two separate cycles, with no vertices in common; (b) there are two cycles with a single vertex in common; (c) there are two special vertices joined by three distinct paths.

In case (a), connectivity implies that there is a path connecting the two cycles. Every edge of this path is a leafless bridge, so Theorem 7 shows that d is not D-optimal.

In case (b), the single vertex in common to the two cycles is a cut-vertex. If d is D-optimal, then Theorem 8 shows that no treatment-vertex is a cut-vertex of \tilde{G} . So suppose that Γ is a block whose vertex is a cut-vertex of \tilde{G} , cutting it into components H_1 and H_2 both containing Γ . Suppose further that both H_1 and H_2 contain other block-vertices in addition to Γ . Theorem 7 shows that neither H_1 nor H_2 contains a leafless bridge, so all of their block-vertices are contained in cycles. By Lemma 1, each component has a single cycle containing all its block-vertices. Figure 16 shows an example, excluding the treatment-vertices outside the cycles. For $m = 1, 2$, let b_m be the number of block-vertices in H_m in addition to Γ . Thus $b = b_1 + b_2 + 1 \geq 3$, and H_m contains $2(b_m + 1)$ spanning trees, each made by omitting one edge from its cycle. Thus the number of spanning trees of \tilde{G} is $4(b_1 + 1)(b_2 + 1)$. This is maximized when b_1 and b_2 are as equal as possible. If $b = 2n + 1$, then it is maximized at $(b + 1)^2$ when $b_1 = b_2 = n$; if $b = 2n + 2$, then it is maximized at $b(b + 2)$ when b_1 and b_2 are equal to n and $n + 1$ in either order.

In case (c) there are two special vertices W_1 and W_2 in \tilde{G} which are joined by three disjoint paths. Because there are no bridges, every block-vertex is either one of W_1 and W_2 or is contained in a single path. If W_1 and W_2 are both block-vertices, then the path lengths are all even and sum to $2b + 2$. Figure 17 shows an example, excluding the treatment-vertices outside the cycles. If W_1 and W_2 are both treatment-vertices, then the path lengths are all even and sum to $2b$; otherwise, the path lengths are all odd and sum to $2b + 1$.

Denote these path lengths by p_1, p_2 and p_3 . Then the number of spanning trees in \tilde{G} is $p_1 p_2 + p_1 p_3 + p_2 p_3$. This is maximized when $p_1 + p_2 + p_3 = 2b + 2$, so that W_1 and W_2 are both block-vertices, and the path lengths are as equal as possible. If $b = 3m + 1$, this happens when two of the path lengths are $2m + 2$ and the other is $2m$; if $b = 3m + 2$, it happens when all of the path lengths are $2m + 2$; if $b = 3m + 3$, it happens when two of the path lengths are $2m + 2$ and the other is $2m + 4$. In every case, $p_1 p_2 + p_1 p_3 + p_2 p_3 > (b + 1)^2$, so a design with a block cut-vertex cannot be D-optimal. A D-optimal design can be constructed by drawing a graph with three paths, of the prescribed lengths, between block-vertices W_1 and W_2 ; inserting one treatment in alternate vertices in each path (and hence in the two blocks on either

Fig. 16 An example of the cycles in the Levi graph in the second case in Sect. 5.3, with $b_1 = 5$ and $b_2 = 4$

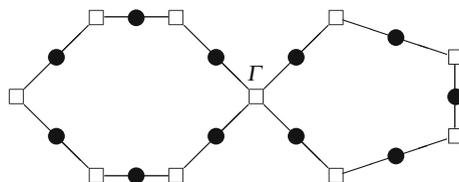
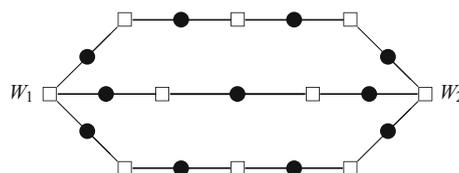


Fig. 17 An example of the cycles of the Levi graph in the third case in Sect. 5.3, with $p_1 = p_3 = 8$ and $p_2 = 6$



side); inserting $k - 3$ other treatments into the blocks with vertices W_1 and W_2 ; and inserting $k - 2$ other treatments into every other block. This works whenever $k \geq 3$.

For $k = 2$, it is not possible for either of W_1 or W_2 to be a block-vertex. A similar argument shows that, in this case, the D-optimal designs are made by allocating two treatments to these vertices, drawing three paths of the prescribed lengths between them, and inserting one block in alternate vertices in each path.

This result was given in [7].

For example, when $b = 10, k = 4$ and $v = 29$, then the non-leaf part of the Levi graph is as shown in Fig. 17. If vertices W_1 and W_2 represent blocks 1 and 10, respectively, one possibility for the D-optimal design is shown in Fig. 18. On the other hand, if $b = 11, k = 2$ and $v = 10$, then we need to swap the roles of treatment-vertices and block-vertices in Fig. 17. Figure 19 shows one possibility for the D-optimal design in this case.

6 A-optimal Block Designs with Low Cycle Rank

6.1 Minimal Number of Observations

Theorem 14 *If $bk = b + v - 1$, then a block design for v treatments in b blocks of size k is A-optimal if and only if there is one treatment that occurs in every block.*

Proof As in the proof of Theorem 12, if the Levi graph is connected, then it must be a tree. Every non-leaf vertex of a tree is a cut-vertex, so Theorem 10 shows that all treatment-vertices but one are leaves, so these treatments have replication 1. Connectivity then implies that the remaining treatment is in every block. The converse follows from the fact that the Levi graph of each block design that has one treatment that occurs in each block has the same sum of resistance distances. \square

Designs like those in Theorem 14 are called *star designs* in [3], and *queen-bee designs* in [4]. Figure 20 shows an example with $b = 8, k = 4$ and $v = 25$.

Theorem 14 was proved in [3,8,25]. Now the groundwork in Sect. 4 makes the proof simpler.

1	1	2	3	5	6	8	9	10	4
5	2	3	4	6	7	9	10	11	7
8	13	15	17	19	21	23	25	27	11
12	14	16	18	20	22	24	26	28	29

Fig. 18 A D-optimal block design with $b = 10, k = 4$ and $v = 29$

1	2	3	4	1	5	6	1	7	8	9
2	3	4	10	5	6	10	7	8	9	10

Fig. 19 A D-optimal block design with $b = 11, k = 2$ and $v = 10$

6.2 Nearly Minimal Number of Observations

As noted in Sect. 5.2, if $c = 1$, then $v = b(k - 1)$ and the Levi graph contains a single cycle. Let s be the number of block-vertices in this cycle. Then the cycle contains s treatment-vertices and $2s$ edges. If $s = b$, then there are no cut-vertices. If $1 < s < b$, then there is at least one block-vertex outside the cycle. If the path joining it to the cycle meets the cycle in a block-vertex, then that path contains a treatment-vertex which is not in a cycle and is a cut-vertex: by Theorem 11, the design is not A-optimal. On the other hand, if that path meets the cycle in a treatment-vertex ℓ , then that vertex is a cut-vertex. Theorem 10 shows that if the block design is A-optimal, then there is no other treatment cut-vertex. Hence treatment-vertex ℓ is joined to all the $b - s$ block-vertices outside the cycle. If $s = 1$, then the treatment whose vertex is in the cycle occurs twice in the block whose vertex is in the cycle, so connectivity implies that $k \geq 3$. Denote by $\mathcal{C}(b, k, s)$ the set of block designs satisfying these conditions.

Figures 2 and 3 show the Levi graphs of block designs in $\mathcal{C}(6, 4, 6)$ and $\mathcal{C}(6, 4, 3)$, respectively.

Lemma 3 *Suppose that $v = b(k - 1)$ and a block design is in $\mathcal{C}(b, k, s)$. Then the sum of all the pairwise resistance distances between treatment-vertices in the Levi graph is $g(s)/6$, where*

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

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

Proof Let \mathcal{V}_1 be the set of treatment-vertices in the cycle, let \mathcal{V}_2 be the set of other treatment-vertices joined to block-vertices in the cycle, and let \mathcal{V}_3 be the set of remaining treatment-vertices. Suppose that i and j are in \mathcal{V}_1 , with $i \neq j$. The two paths from i to j have lengths $2p$ and $2(s - p)$ for some p with $1 \leq p \leq s - 1$. The rule for combining resistance distances in parallel gives

$$R_{ij} = \left(\frac{1}{2p} + \frac{1}{2(s - p)} \right)^{-1} = \frac{2p(s - p)}{s}.$$

For each fixed i , the sum of R_{ij} as j varies over \mathcal{V}_1 is

$$\sum_{p=1}^{s-1} \frac{2p(s - p)}{s} = \frac{(s - 1)(s + 1)}{3}.$$

1	1	1	1	1	1	1	1
2	5	8	11	14	17	20	23
3	6	9	12	15	18	21	24
4	7	10	13	16	19	22	25

Fig. 20 An A-optimal block design with $b = 8, k = 4$ and $v = 25$

Call this P_1 . If Γ is a block-vertex in the cycle, then the same argument shows that the sum of the resistance distances from Γ to other block-vertices in the cycle is also equal to P_1 .

Similarly, if i and Γ are a treatment-vertex and block-vertex in the cycle, then the two paths from i to Γ have lengths $2q - 1$ and $2s - 2q + 1$ for some q with $1 \leq q \leq s$. For each fixed i , the sum of $R_{i\Gamma}$ as Γ varies over these blocks is

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

Call this P_2 .

For $1 \leq m \leq n \leq 3$, denote by \mathcal{R}_{mn} the sum of the pairwise resistance distances between vertices in \mathcal{V}_m and \mathcal{V}_n . Thus $\mathcal{R}_{11} = sP_1/2$.

Suppose that vertex t in \mathcal{V}_2 is joined to block-vertex Γ . If $i \in \mathcal{V}_1$, then the rule for combining resistance distances in series gives $R_{ti} = R_{t\Gamma} + R_{\Gamma i} = 1 + R_{\Gamma i}$. Summing over i in \mathcal{V}_1 gives $s + P_2$. There are $s(k - 2)$ vertices in \mathcal{V}_2 , and so $\mathcal{R}_{12} = s(k - 2)(s + P_2)$.

Let t and u be distinct vertices in \mathcal{V}_2 . If they are joined to the same block-vertex, then $R_{tu} = 2$. There are $s(k - 2)(k - 3)/2$ such pairs, so the sum of these resistance distances is $s(k - 2)(k - 3)$. If they are joined to different block-vertices Γ and Δ , then $R_{tu} = 2 + R_{\Gamma\Delta}$. There are $(k - 2)^2$ such pairs for each choice of Γ and Δ , so the sum of these resistance distances is $(k - 2)^2[s(s - 1) + \mathcal{R}_{11}]$. Hence $\mathcal{R}_{22} = s(k - 2)(k - 3) + s(s - 1)(k - 2)^2 + s(k - 2)^2 P_1/2$.

If $t \in \mathcal{V}_3$ and $u \in \mathcal{V}_1 \cup \mathcal{V}_2$, then $R_{tu} = 2 + R_{\ell u}$, where ℓ is the cut-vertex. Summing over u in \mathcal{V}_1 gives $2s + P_1$, while summing over u in \mathcal{V}_2 gives $(k - 2)(3s + P_2)$. There are $(b - s)(k - 1)$ vertices in \mathcal{V}_3 , and so $\mathcal{R}_{13} = (b - s)(k - 1)(2s + P_1)$ and $\mathcal{R}_{23} = (b - s)(k - 1)(k - 2)(3s + P_2)$.

If different vertices t and u in \mathcal{V}_3 are in the same block, then $R_{tu} = 2$; otherwise, $R_{tu} = 4$. Hence $\mathcal{R}_{33} = (b - s)(k - 1)(k - 2) + 2(b - s)(b - s - 1)(k - 1)^2$.

Adding $\mathcal{R}_{11}, \mathcal{R}_{12}, \mathcal{R}_{13}, \mathcal{R}_{22}, \mathcal{R}_{23}$ and \mathcal{R}_{33} shows that the sum of all the pairwise resistance distances between treatment-vertices in the Levi graphs is $g(s)/6$. \square

Theorem 15 *If $v = b(k - 1)$, then a block design for v treatments in b blocks of size k is A -optimal if and only if it is in $\mathcal{C}(b, k, s)$, where*

- (i) $s = b$ if $2 \leq b \leq 4$, or $b = 5$ and $k \leq 5$, or $b = 6$ and $k \leq 3$, or $7 \leq b \leq 8$ and $k = 2$;
- (ii) $s = 4$ if $9 \leq b \leq 11$ and $k = 2$;
- (iii) $s = 3$ or $s = 4$ if $b = 12$ and $k = 2$;
- (iv) $s = 3$ if $b = 6$ and $k = 4$, or $7 \leq b \leq 11$ and $k = 3$, or $b \geq 13$ and $k = 2$;
- (v) $s = 2$ otherwise.

Proof Lemma 3 shows that we need to find the value of s , for s in $\{1, 2, \dots, b\}$, which minimizes $g(s)$. First, we note that

$$\begin{aligned} g(1) - g(2) &= 7(k - 1)^2 - 6b(k - 1)^2 + 6bk(k - 1) - 4k^2 + 2k - 1 \\ &= (3k + 6b - 9)(k - 1) - 3 > 0, \end{aligned}$$

because $b \geq 2$ and $k \geq 2$. Thus designs in $\mathcal{C}(b, k, 1)$ are never A-optimal.

We now take four steps to find the integer s in $[2, b]$ which minimizes $g(s)$.

Step 1 If we regard the polynomial function g as defined on the real numbers, then

$$g'(s) = -3(k - 1)^2s^2 + 4b(k - 1)^2s - 6bk(k - 1) + 4k^2 - 2k + 1.$$

This is zero when

$$s = \frac{2b}{3} \pm \frac{(k - 1)\sqrt{\alpha(b, k)}}{3(k - 1)^2},$$

where

$$\alpha(b, k) = 4b^2(k - 1)^2 - 18bk(k - 1) + 12k^2 - 6k + 3.$$

If $\alpha(b, k) < 0$, then $g'(s)$ is never zero for real values of s , and so $g(s)$ decreases monotonically. Thus $g(s)$ is minimized for $s \in \{1, 2, \dots, b\}$ at $s = b$. This happens for all k when $b = 2$ or $b = 3$, and for $k \leq 14$ when $b = 4$. When $b = 4$, then $g(3) - g(4) = k^2 + 16k - 20 > 0$ for all $k \geq 2$, so $g(s)$ is minimized for $s \in \{1, 2, 3, 4\}$ at $g(4)$.

It is also the case that $\alpha(b, k) < 0$ if $b = 5$ and $k \leq 4$; if $b = 6$ and $k \leq 3$; and if $b = 7$ and $k = 2$. In all of these cases, $g(s)$ is minimized for $s \in \{1, 2, \dots, b\}$ at $s = b$.

From now on, we may assume that $b \geq 5$.

Step 2 Now we compare $g(b)$ with $g(2)$ and $g(3)$, and show that $g(b)$ is larger than at least one of the other two in almost all of the remaining cases. We have

$$g(b) - g(2) = b^2(k - 1)[(b - 6)(k - 1) - 6] + b(8k^2 - 7) + 2k(b - 6) + 6.$$

If $b = 5$, this is $15k^2 - 102k + 96$, which is positive whenever $k \geq 6$. If $b = 6$, it is $12(4k^2 - 18k + 15)$, which is positive whenever $k \geq 4$. For all larger values of b , it is positive whenever $k \geq 3$.

When $k = 2$,

$$g(b) - g(3) = b^2(b - 12) + 31b - 12.$$

This is positive whenever $b \geq 9$.

Thus $g(b)$ does not give the minimum value if $k \geq 6$ and $b \geq 5$, if $k \geq 4$ and $b \geq 6$, if $k \geq 3$ and $b \geq 7$, or if $k = 2$ and $b \geq 9$. In all these cases, it suffices to find the real number s_0 in $(1, b]$ where $g'(s_0) = 0$; note that $s_0 \neq 1$, because $g(1) > g(2)$. If $s_0 < 2$, then the minimum for integer s occurs at $s = 2$. Otherwise, if s_0 is not an integer, compare $g(s_1)$ and $g(s_2)$, where s_1 and s_2 are the integers on either side of s_0 .

Step 3 If $g(3) > g(2)$, then the overall minimum of $g(s)$ on $[1, b]$ occurs in $[1, 3]$, and the minimum value for integer s is at $s = 2$. Now,

$$g(3) - g(2) = (4bk - 10b - 15k + 21)(k - 1) + 3.$$

This is always negative when $k = 2$. However, $g(3) - g(2) > 0$ when $k = 3$ and $b \geq 12$; when $k = 4$ and $b \geq 7$; when $k = 5$ and $b \geq 6$; and when $k \geq 6$ and $b \geq 5$. Apart from the situation with $k = 2$, this leaves only a small finite number of cases to be checked.

Step 4 When $k = 2$, $g(s) = -s^3 + 2bs^2 - (12b - 13)s + C$. Therefore $g(4) - g(3) = 2b - 24$. Hence the minimum occurs at $s = 3$ if $b \geq 13$. If $b = 12$, then $g(3) = g(4)$ and the minimum value for integers s occurs at both points. If $b \leq 11$, then $g(s)$ is minimized for some s in $[4, b]$. From Step 1, the only remaining cases to check are values of b with $8 \leq b \leq 11$. \square

For example, this theorem shows that the block design in Fig. 1(b) is A-optimal.

Theorem 15 was proved in [4,22,31]. Again, the proof here is much shorter (in spite of the detailed calculations) now that we have the groundwork in Sect. 4.

Theorems 13 and 15 show that, for $c = 1$, the A-optimal designs are very different from the D-optimal designs as either of b or k increases.

7 Comments and Conclusions

7.1 Summary

In this paper, we have concentrated on using properties of the Levi graph to find the D-optimal block designs and A-optimal block designs when the number of observations is close to minimal. We believe that the results in Sect. 4 are new. Moreover, they do not depend on the number of observations being small. They show that, if the cycle rank is at least 1, then the Levi graph of a D-optimal design does not contain any bridge, except, possibly, one whose treatment-vertex is a leaf. Moreover, in the Levi graph of a D-optimal design with cycle rank at least 1, no treatment-vertex is a cut-vertex. The Levi graph of an A-optimal design with cycle rank at least 1 can have no more than one treatment-vertex which is a cut-vertex, and any such vertex must be contained in a cycle.

Sections 5 and 6 use the results of Sect. 4 to give unified, and shorter, proofs of a number of known results about D-optimal and A-optimal designs with low cycle rank. Parts of [4] referred to a preliminary version of the current paper for details of the proofs.

For small designs with cycle rank 1, the same design can be both D-optimal and A-optimal. For example, when $b = k = 4$ and $v = 16$, then the design in Fig. 21 is D-optimal, by Theorem 13, and A-optimal, by Theorem 15.

However, as the number of treatments increases, the A-optimal designs diverge from the D-optimal designs. For example, when $b = 6$, $k = 4$ and $v = 18$, then

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

Fig. 21 A block design with $b = k = 4$ and $v = 12$ which is both D-optimal and A-optimal

the design in Fig. 1a is D-optimal, by Theorem 13, but the design in Fig. 1b is A-optimal, by Theorem 15. The geometric means of the non-trivial eigenvalues of the information matrices of these two designs are 0.8411 and 0.8075, respectively. Their harmonic means are 0.5829 and 0.6000, respectively.

7.2 What About Dual Designs?

If d is a block design, then its *dual* block design d^\top is made by simply interchanging the roles of treatments and blocks. In the case that all treatments have the same replication, in addition to all blocks having the same size, John and Mitchell proved in [18] that d^\top is D-optimal if and only if d is D-optimal, and that d^\top is A-optimal if and only if d is A-optimal. Thus if we are interested in estimating block effects, and use equireplicate designs, then the designs which are optimal for block effects are the same as those which are optimal for treatment effects, under either the D or the A criterion.

In most experimental situations, both management constraints and randomization concerns lead us to use blocks of equal size, even though there is no such restriction on treatment replication. We are not usually interested in estimating block effects, so we are not concerned about the optimality of d^\top . Suppose that we are interested in block effects, as well as treatment effects. Since the Levi graph of d^\top is the same as the Levi graph of d , Theorem 3 shows that d^\top is D-optimal if and only if d is D-optimal. Thus, whether or not we insist on equal replication for treatments, the design which is D-optimal for treatment effects is D-optimal for block effects.

The same is true for A-optimality when the cycle rank is 0. Theorem 14 shows that the A-optimal designs are precisely the star designs. The dual of a star design has one complete block, and all other blocks of size one. Therefore a star design gives the minimal sum of resistance distances between pairs of block-vertices.

However, the same is not true for A-optimality in general. For example, consider cycle rank 1. When $k = 2$ and $b = v$, an investigation like the one in the proof of Theorem 15 shows that, for $b \geq 5$, d^\top is A-optimal if and only if d is in $\mathcal{C}(b, 2, 2)$.

7.3 What About Larger Cycle Rank?

It seems unlikely that the detailed investigations in Sects. 5 and 6 can be replicated for larger cycle ranks. However, Section 6 of [1] does suggest that, when average replication is no more than three, the A-optimal designs will diverge from the D-optimal designs as v increases. Thus John and Mitchell's assumption in [18] that optimal designs will always be equireplicate if possible is no longer tenable. We recommend that any computer search for optimal block designs should not rule out considering designs with unequal (possibly very unequal) replication of treatments.

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