Optimal BIBD-extended designs

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Abstract

Balanced incomplete block designs (BIBDs) are a class of designs with \( v \) treatments and \( b \) blocks of size \( k \) that are optimal with regards to a wide range of optimality criteria, but it is not clear which designs to choose for combinations of \( v \), \( b \) and \( k \) when BIBDs do not exist.

In 1992, Cheng showed that for sufficiently large \( b \), the designs which are optimal with respect to commonly used criteria (including the \( A \)- and \( D \)- criteria) must be found among \((M.S)\)-optimal designs. In particular, this result confirmed the conjecture of John and Mitchell in 1977 on the optimality of regular graph designs (RGDs) in the case of large numbers of blocks.

We investigate the effect of extending known optimal binary designs by repeatedly adding the blocks of a BIBD and find boundaries for the number of block so that these BIBD-extended designs are optimal. In particular, we will study the designs for \( k = 2 \) and \( b = v - 1 \) and \( b = v \): in these cases the \( A \)- and \( D \)-optimal designs are not the same but we show that this changes after adding blocks of a BIBD and the same design becomes \( A \)- and \( D \)-optimal amongst the collection of extended designs. Finally, we characterise those RGDs that give rise to \( A \)- and \( D \)-optimal extended designs and extend a result on the \( D \)-optimality of the a group-divisible design to \( A \)- and \( D \)-optimality amongst BIBD-extended designs.

Keywords — \( A \)-optimality, \( D \)-optimality, Incomplete block design, Regular graphs, Regular graph design, BIBD-extended design

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1 Introduction and Preliminaries

One of the main questions in the theory of optimal designs is how to design experiments for the comparison of treatments when the available experimental units are also affected by other nuisance or blocking factors. The blocking factors are usually of no experimental interest, however they influence the measurements of the treatment responses and must be accounted for in the experimental design. Specifically, suppose there are $v$ treatments to be compared on a number of experimental units that can be partitioned into $b$ blocks of size $k$ with $k < v$. These blocks might differ systematically but all units in a block are assumed to be alike. To each unit, one of the treatments will be applied, after which the response of the unit is measured. This assignment of treatments to the blocked experimental units is called a block design. Since we are interested in the comparison of treatments, rather than estimating the response of a single treatment, we estimate a set of treatment contrast, that is a linear combination of the treatment effects whose coefficients sum up to zero. The variances of estimators of the unknown parameters are a function only of the treatment-unit assignment and can be calculated (up to a scalar multiple) before any measurements are taken. Therefore, the design optimality question often is the search for a treatment-unit assignment so that the estimate has the least possible variance. This can be a multidimensional problem and a design can be deemed good in different ways.

We give the basic definitions in the following and the reader is referred to [SS89] for numerous references and [BC09] where more details on the application of combinatorics in the theory of design of experiments can be found. We will assume that both treatment and blocking factors affect the mean response additively, and that responses are otherwise subject to equivariable noise that is uncorrelated from one unit to another. If all pairwise differences are estimable, the design is said to be connected. The design is called binary, if every treatment occurs at most once per block. We will always assume the designs to be binary and that $k < v$ (but not necessarily connected). The replication $r_i$ of a treatment $i$ is the total number of units that have been assigned treatment $i$, and if the replications are all equal to a constant $r$, the design is called equireplicate. Let $N_d$ be the $v \times b$ treatment-block incidence matrix of the design $d$, i.e. the $ij$-entry of $N_d$ is the number of units in block $j$ that have been assigned treatment $i$. The concurrence of treatments $i$ and $j$ is the $ij$-entry of the product $N_d N_d^T$ and will be denoted by $\lambda_{ij}$. For binary designs, $\lambda_{ii} = r_i$ and $\lambda_{ij}$ is the number of blocks containing both treatments $i$ and $j$. The information matrix for the estimation of the treatment effects is

$$C_d = \text{diag}(r_1, \ldots, r_v) - \frac{1}{k} N_d N_d^T.$$  

Since $C_d$ has row sums 0, the all-1-vector is an eigenvector with eigenvalue 0. All other eigenvalues, the non-trivial eigenvalues, are positive. If the design is connected, the rank of the information matrix is $v - 1$, the eigenvalue 0 has multiplicity 1 and all non-trivial eigenvalues are strictly positive. The Laplacian
Matrix of a binary connected design is
\[ L_d = k \text{diag}(r_1, \ldots, r_v) - N_d N_d^T = kC_d. \]

The smallest eigenvalue of \( L_d \) is 0 and the other \( v - 1 \) non-trivial Laplacian eigenvalues are all positive (and strictly positive if the design is connected). The non-zero eigenvalues of \( C_d \) are the reciprocals of the variances for a set of orthonormal treatment contrasts (aside from the variance of the noise). Therefore, we can define measures how good a treatment-unit assignment (or design) is based on summary functions of the non-trivial eigenvalues: The average variance of the set of the best linear unbiased estimators of the pairwise differences of the treatment effects is proportional to the reciprocal of the harmonic mean of the non-trivial eigenvalues of \( C_d \), and a design \( d \) that minimizes this summary function is said to be \( A \)-optimal. The volume of the confidence ellipsoid for any orthonormal contrasts is proportional to the product of the reciprocals of the non-zero eigenvalues of \( C_d \), and a design \( d \) that minimizes this product is said to be \( D \)-optimal. There are many more optimality criteria; another popular example is the \( E \)-criterion which is the maximization of the smallest non-trivial eigenvalue of \( C_d \) and is equivalent with minimizing the largest variance of the estimators. A design that maximises the sum of the non-trivial eigenvalues and minimizes the sum of squares of the entries of the information matrix (among those that maximise the sum of the non-trivial eigenvalues) is called \( (M.S) \)-optimal [EH74]. However, the \( (M.S) \)-optimal designs are not unique in their class and often not efficient on the other optimality criteria. If they exist, RGDs are \( (M.S) \)-optimal [Che92]. A design is called Schur-optimal if the non-trivial eigenvalues of \( C_d \) majorize the non-trivial eigenvalues of the information matrix of any competing design. Schur-optimality is a most general optimality criterion: a Schur-optimal design minimizes any Schur-convex function of the non-trivial Laplacian eigenvalues, that is any function such that, if \( x \in A \subseteq \mathbb{R}^n \) is majorized by \( y \in A \) then \( \Phi(x) \geq \Phi(y) \), whenever \( x \) is not a permutation of \( y \); examples of Schur-convex functions are the \( A \)-, \( D \)- and \( E \)-criteria. Discussions of these and other optimality criteria can be found in [SS89].

There is no general answer to the question of which design is to be chosen for given \( v, b \) and \( k \), but there are several partial results for certain choices of \( v, b \) and \( k \): balanced incomplete block designs (in short BIBDs) are binary equireplicate incomplete block designs with replication \( bk/v \), where \( k < v \) and any pair of treatments is contained in exactly \( \lambda \) blocks for some \( \lambda > 0 \). BIBDs are optimal with regards to a wide range of criteria, in particular the \( A \)- and \( D \)-criteria [Kie75], but it is not clear which designs to choose if no BIBD exists. Other popular designs are the regular graph designs (in short RGDs): these are equireplicate binary designs in which any pair of points occurs in either \( \lambda \) or \( \lambda + 1 \) blocks for some integer \( \lambda \geq 0 \). The Laplacian matrix of an RGD \( d \) with \( v \) treatments, replication \( r \) and block size \( k \) can be written as
\[ L_d = (r(k - 1) + \lambda)I_v - T_d - \lambda J_v, \]
where \( I_v \) is the \( v \times v \) identity matrix, \( J_v \) denotes the \( v \times v \) all-1-matrix and \( T_d \) is a symmetric \( v \times v \) \((0,1)\)-matrix with 0’s on the diagonal and exactly
$r(k - 1) - \lambda(v - 1)$ number of 1’s in each row and each column. Note that the Laplacian matrix of an RGD is therefore fully determined by the parameters $v$, $k$, $r$ and the matrix $T_d$.

The reference to graphs in the names of the RGDs is hinting towards a close relationship between block designs and graphs that hinges on the notion of the Laplacian matrix. First, we will need some basic definitions: a graph $\mathcal{G}$ is a set of $v$ vertices and a set of edges that connect vertices $i \neq j$ (we do not allow any loops). The adjacency matrix $A_\mathcal{G}$ of the graph $\mathcal{G}$ is the $v \times v$ matrix whose $ij$-entry is the number of edges joining vertices $i$ and $j$. A graph $\mathcal{G}$ is connected if any vertex can be reached from any other vertex by going along edges. We say that $\mathcal{G}$ is simple, if $\mathcal{G}$ contains no multiple edges. The degree $\delta_i$ of the vertex $i$ is the number of edges incident to $i$. If the degrees of all its vertices are equal to a constant $\delta$, the degree of the graph, the graph is called regular (note that its adjacency matrix has constant row and column sums).

The Laplacian matrix $L_\mathcal{G}$ of a graph $\mathcal{G}$ on $v$ vertices is defined as

$$L_\mathcal{G} = \text{diag}(\delta_1, \ldots, \delta_v) - A_\mathcal{G}.$$  

Note that $L_\mathcal{G}$ is a symmetric matrix with row and column sums zero. A binary block design can be represented as a graph, called the concurrence graph, by taking the treatments as vertices and joining any two distinct vertices $i$ and $j$ are joined by $\lambda_{ij}$ edges, where $\lambda_{ij}$ is the concurrence of $i$ and $j$. Note that the concurrence graph contains no loops, even if the design is not binary, but is not necessarily simple. If $\mathcal{G}$ is the concurrence graph of a binary design $d$ with block size $k$, then $\delta_i = r_i(k - 1)$, $i = 1, \ldots, v$ and then $L_\mathcal{G} = L_d$.

All regular simple graphs with $v$ vertices of degree $\delta$ correspond to all symmetric $v \times v$-matrices with (0, 1)-entries, zero diagonal and row and column sum $\delta$; that is the matrix $T_d$ of a RGD $d$ is precisely the adjacency matrix of a simple regular graph of degree $r(k - 1) - \lambda(v - 1)$. John and Mitchell conjectured that if an incomplete block design is $D$-optimal (or $A$-optimal or $E$-optimal), then it is an RGD (if any RGDs exist) [JM77]. This conjecture has been shown to be wrong for all three optimality criteria [JE80; Con86; Bai07], but holds if the number of blocks is large enough [Che92].

In this context, we want explore the boundaries of when RGDs become optimal and the landscape of optimal designs with a large number of blocks. In particular, we are interested in the effect of adding the blocks of a BIBD repeatedly to a design on the performance of the design on the $A$- and $D$-criteria (for a treatment of the $E$-criterion see [Mor07]). In the spirit of [Mor07], we call these designs BIBD-extended designs. We will define a partial order on the Laplacian matrices and identify some bounds on the number of blocks for which BIBD-extended RGDs are $A$- and $D$-optimal among all competing BIBD-extended binary designs in Section 2. We will use these bounds in Section 3 to prove the $A$- and $D$-optimality of some of the BIBD-extended designs. In Section 4 we will identify some bounds on the number of blocks for which a class of BIBD-extended RGDs are $A$- and $D$-optimal among BIBD-extended RGDs and use these to prove the $A$- and $D$-optimality of certain BIBD-extended group-divisible designs among BIBD-extended RGDs.
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2 A partial order on BIBD extended designs and $A$- and $D$-optimality

Suppose, the binary design $d$ has Laplacian matrix $L_d$ and $\tilde{d}$ is a BIBD on $v$ treatments and block size $k$ with $b$ blocks and Laplacian matrix $L_{\tilde{d}}$ and concurrence parameter $\tilde{\lambda}$. Then for $y \in \mathbb{N}$ the matrix $L_d + yL_{\tilde{d}}$ is the Laplacian matrix of a BIBD-extended design on $v$ points, replication $r + y\lambda(v-1)/(k-1)$ and $b + yb$ blocks of size $k$. Let $\rho_{1d}, \ldots, \rho_{vd-1}$ be the non-trivial Laplacian eigenvalues of $d$, then the BIBD-extended design has the non-trivial eigenvalues $vy + \rho_{1d}, \ldots, vy + \rho_{vd-1}$. We can write the $A$- and $D$-value as functions that only depend on $y$ and $L_d$ as

$$A(y, L_d) := \frac{v - 1}{\sum_{i=1}^{v-1} (vy + \rho_{1d})}$$
and

$$D(y, L_d) := \prod_{i=1}^{v-1} (vy + \rho_{1d}),$$

respectively.

For $z = (z_1, \ldots, z_{v-1}) \in \mathbb{R}^{v-1}$ and $\mathcal{I} = \{1, \ldots, v-1\}$, let

$$S_0(z) \equiv 1 \text{ and } S_j(z) := \sum_{\substack{\mathcal{J} \subseteq \mathcal{I} \setminus \{j\} \mid |\mathcal{J}| = j}} \prod_{i \in \mathcal{J}} z_i.$$ $S_j$ is called the $j$th elementary symmetric polynomial. Then for $\rho^{L_d} := (\rho_{1d}, \ldots, \rho_{vd-1})$ [Cak17]

$$D(y, L_d) = \sum_{j=0}^{v-1} (vy)^{v-1-j} S_j(\rho^{L_d}), \text{ and}$$

$$A(y, L_d) = \frac{(v - 1) \sum_{j=0}^{v-1} (vy)^{v-1-j} S_j(\rho^{L_d})}{\sum_{j=0}^{v-2} (vy)^{v-2-j}(v - 1 - j)S_j(\rho^{L_d})}.$$ (2.1)

Note that the $A$-value is a rational function whose coefficients are completely determined by the coefficients of the $D$-value and $\rho_{1d}, \ldots, \rho_{vd-1}$ are also the Laplacian eigenvalues of the concurrence graph, $\mathcal{G}_d$ of $d$. For $j \in \{1, \ldots, v-1\}$, there exists a relationship between $S_{v-j}(\rho^{L_d})$ and the set $\mathcal{F}_j$ of all disjoint unions $F_j$ of $j$ subgraphs of $\mathcal{G}$ on $n_1, \ldots, n_j$ vertices in which any two vertices are connected by exactly one path (for example [CDS79], p. 38):

$$S_{v-j} = \sum_{F_j \subseteq \mathcal{F}_j} \gamma(F_j),$$
where \( \gamma(F_j) = \prod_{k=1}^v n_k \) for all \( F_j \in \mathcal{F}_j \). In particular, \( S_j(\rho^{L_i}) \in \mathbb{N}_{>0} \) for \( j = 1, \ldots, v \).

Because the performance of a BIBD-extended binary design on the \textit{A}- and \textit{D}-criteria is in this way closely related to the elementary symmetric polynomials of its non-trivial Laplacian eigenvalues, we want to define an order on the matrices accordingly. We will do this in a similar fashion to \cite{Con86} and take the lexicographic ordering corresponding to the elementary symmetric polynomials of the non-trivial eigenvalues of the Laplacian matrices. That means, for two Laplacian matrices \( L, L' \in \mathcal{L}(v, b, k) \) whose set of eigenvalues do not coincide, we will write \( L' \prec L \) if there exists an \( l \in \{1, \ldots, v-1\} \) such that

\[
S_l(\rho^{L'}) < S_l(\rho^L) \quad \text{and} \quad S_j(\rho^{L'}) = S_j(\rho^L) \quad \text{for} \quad j = 1, \ldots, l-1.
\]

This is a reflexive and transitive relation which we will call the \textit{stable order} on \( \mathcal{L}(v, b, k) \). Note that matrices are indistinguishable in this order if they have the same eigenvalues. From Equation (25) it is immediately clear that if \( L' \prec L \), then there exists a \( y_0 \geq 0 \) such that \( D(y, L') \leq D(y, L) \) for \( y \geq y_0 \). If \( L' \prec L \) such that \( l \) is the smallest index with \( S_l(\rho^{L'}) - S_l(\rho^L) \neq 0 \), then the polynomial

\[
P(y, L, L') := \sum_{i=1}^{2v-3} p_i y^i = \sum_{j=0}^{v-1} (vy)^{v-1-j} S_j(\rho^{L'}) \sum_{j=0}^{v-2} (vy)^{v-2-j} (v-1-j) S_j(\rho^{L'})
\]

\[
- \sum_{j=0}^{v-1} (vy)^{v-1-j} S_j(\rho^{L'}) \sum_{j=0}^{v-2} (vy)^{v-2-j} (v-1-j) S_j(\rho^{L'})
\]

has coefficients

\[
p_{2v-3-i} = v^{2v-3-i} \sum_{j=0}^{i} (v-1-j) \left[ S_j(\rho^{L'}) S_{i-j}(\rho^L) - S_j(\rho^L) S_{i-j}(\rho^{L'}) \right]
\]

that are equal to zero for \( i = 1, \ldots, l-1 \), and the first non-vanishing coefficient is

\[
p_{2v-3-l} = v^{2v-3-l} \left[ S_l(\rho^L) - S_l(\rho^{L'}) \right] \in \mathbb{N}_{>0}.
\]

Since \( P(y, L, L') \geq 0 \) implies \( A(y, L') \leq A(y, L) \) (Equation (22)), it follows that there exists a \( y_0 \geq 0 \) such that \( A(y, L') \leq A(y, L) \) for \( y \geq y_0 \).

**Corollary 2.1.** For given \( v, b, k \), there exists a \( y_0 \geq 0 \) such that, if designs with Laplacian matrix \( L[y] \) exist for some \( L \in \mathcal{L}(v, b, k) \) and \( y \geq y_0 \), then their order under the \textit{A}- or \textit{D}-criterion is the stable order of the matrices \( L \).

For \( i = 1, \ldots, v-1 \), we will denote by \( \mathcal{L}_i(v, b, k) \) the set of Laplacian matrices \( L \in \mathcal{L}(v, b, k) \) such that

\[
S_j(\rho^L) = \max\{S_j(\rho^{L'})|L' \in \mathcal{L}(v, b, k)\} \quad \text{for} \quad j = 1, \ldots, i.
\]
That means, that for \( i \in \{1, \ldots, v-2\} \) and for \( L, L' \in \mathcal{L}_i(v, b, k) \) with \( L' \notin \mathcal{L}_{i+1}(v, b, k) \) we have \( L' \prec L \). All binary designs coincide on \( S_1 \), and hence \( \mathcal{L}_1(v, b, k) \) is the set of the Laplacian matrices of all binary designs \([Kie59]\); \( \mathcal{L}_2(v, b, k) \) is the set of the Laplacian matrices of \((M.S)\)-optimal designs, these are any existing regular graph designs (RGDs) or nearly balanced incomplete block designs (NBDs) \([Che92, CW81]\). We obtain a similar result to that in \([Con86]\).

**Corollary 2.2.** For given \( v, b, k \) and \( 2 \leq j \leq v \), there exists a \( y_0 \geq 0 \) such that, if designs with Laplacian matrix \( L[y] \) where \( L \in \mathcal{L}_j(v, b, k) \) exist for some \( y \geq y_0 \), then they are \( A \)- and \( D \)-optimal among all designs with Laplacian matrices \( L'[y] \) with \( L' \in \mathcal{L}_1(v, b, k) \setminus \mathcal{L}_j(v, b, k) \).

**Lemma 2.3.** Let \( L = (L_{ij}) \in \mathcal{L}_1(v, b, k) \) and \( \rho_{L_1}^{(v)} \geq \ldots \geq \rho_{L_{v-1}}^{(v)} > 0 \), then \( \rho_{L_1}^{(v)} \leq 2b(k-1) \).

**Proof.** \( L \) is the Laplacian matrix of a connected graph with degrees \( \delta_i = r_i(k-1) \) for \( i = 1, \ldots, v \). The Laplacian eigenvalues of a connected graph are bounded from above (for example \([DB05]\)) by \( \max\{\delta_u + \delta_w | (u, w) \in E(G)\} \). Since \( r_i \leq b \), it follows \( \rho_{L_1}^{(v)} \leq \max\{(r_i + r_j)(k-1) | L_{ij} \neq 0, i \neq j\} \leq 2b(k-1) \).

**Lemma 2.4.** The binomial coefficient \( \binom{v}{j} \) (as a function in \( j = 1, \ldots, v-1 \)) is monotone increasing for \( j \leq \lfloor \frac{2v-3}{3} \rfloor \) and attains its maximum at \( \lfloor \frac{2v-3}{3} \rfloor \).

**Proof.** Follows directly from

\[
\frac{2\binom{j+1}{v-1}}{\binom{j}{v-1}} = \frac{2(v-1-j)}{j+1} > 1 \text{ iff } j < \frac{2v-3}{3}, \quad j = 3, \ldots, v-1.
\]

**Lemma 2.5.** The binomial coefficient \( \binom{v}{j} \) as a function in \( j \) is strictly increasing until \( j < \frac{v^2-2}{v^2} \) and the maximum is attained at \( \lfloor \frac{v^2-2}{v^2} \rfloor \).

**Proof.** Follows directly from

\[
\frac{\binom{j+1}{v-1}}{\binom{j}{v-1}} = \frac{v-1-j}{j+1}.
\]

**Proposition 2.6.** Suppose, \( \mathcal{L}_1(v, b, k) \neq \mathcal{L}_2(v, b, k) \).

1. For given \( v, b, k \) and \( y_0 = v^22^m(b(k-1))^{v-1}\binom{v-1}{m} + 1 \), where \( m = \lfloor \frac{2v-3}{v^2} \rfloor \), if there exist designs with Laplacian matrix \( L[y] \) with \( L \in \mathcal{L}_2(v, b, k) \) and \( y \geq y_0 \), then they are \( D \)-optimal among all designs with Laplacian matrix \( L'[y] \) with \( L' \in \mathcal{L}_1(v, b, k) \).
2. For given \( v, b, k \) and \( y_0 = 2^{v-2}(b(k-1))^{v-1}(2v-5)(^v_m)^2 + \frac{1}{v} \), where \( m = \lfloor \frac{v-2}{2} \rfloor \), if there exist designs with \( L[y] \) with \( L \in \mathcal{L}_2(v, b, k) \) and \( y \geq y_0 \), then they are A-optimal among all designs with Laplacian matrix \( L'[y] \) with \( L' \in \mathcal{L}_1(v, b, k) \).

Proof. 1. Let \( m = \lfloor \frac{v-2}{2} \rfloor \). With Lemmas 2.3 and 2.4

\[
|S_j(\rho^L) - S_j(\rho^{L'})| \leq (b(k-1))^j 2^m \left( \frac{v-1}{m} \right).
\]

Since \( S_j(\rho^L) - S_j(\rho^{L'}) \in \mathbb{N} \) for \( j = 1, \ldots, v-1 \), it follows for \( y \geq v^2 2^m (b(k-1))^{v-1}(^v_m)^2 + 1 \) that

\[
\sum_{j=3}^{v-1} y^{v-1-j} |S_j(\rho^L) - S_j(\rho^{L'})| < 2^m (vb(k-1))^{v-1} \left( \frac{v-1}{m} \right) \sum_{j=3}^{v-1} y^{v-1-j}
\]

\[
\leq 2^m (vb(k-1))^{v-1} \left( \frac{v-1}{m} \right) \frac{y^{v-3} - 1}{y - 1}
\]

\[
\leq y^{v-3}(y-1)^{(v-3) - 1} \frac{y^{v-3}}{y - 1}
\]

\[
< y^{v-3} y^{v-3} [S_2(\rho^L) - S_2(\rho^{L'})].
\]

2. Let \( m = \lfloor \frac{v-2}{2} \rfloor \). With Lemmas 2.3 and 2.4 it follows for all \( i = 1, \ldots, v-1 \), that

\[
|S_j(\rho^L)S_{i-j}(\rho^{L'}) - S_j(\rho^{L'})S_{i-j}(\rho^L)| \leq (2b(k-1))^i \left( \frac{v-1}{m} \right)^2, j = 3, \ldots, v-1.
\]

For \( y - \frac{1}{v} \geq 2^{v-2}(b(k-1))^{v-1}(2v-5)(^v_m)^2 \)

\[
\sum_{i=3}^{v-1} (vy)^{2v-3-i} \sum_{j=0}^{i} (v-1-j) \left| S_j(\rho^L)S_{i-j}(\rho^{L'}) - S_j(\rho^{L'})S_{i-j}(\rho^L) \right|
\]

\[
\leq (2b(k-1))^{v-1} \left( \frac{v-1}{m} \right)^2 \sum_{i=3}^{v-1} (vy)^{2v-3-i} \sum_{j=0}^{i} (v-1-j)
\]

\[
= (2b(k-1))^{v-1} \left( \frac{v-1}{m} \right)^2 \sum_{i=3}^{v-1} (vy)^{2v-3-i} (i+1) \frac{2(v-1) - i}{2}
\]

\[
< (2b(k-1))^{v-1} \left( \frac{v-1}{m} \right)^2 v(2v-5) \frac{2(v-1)}{2} (vy)^{2v-6-(v-4)} \sum_{i=0}^{v-4} (vy)^i
\]

\[
< (vy - 1)(vy)^{v-2} \frac{(vy)^{v-3} - 1}{vy - 1}
\]

\[
< 2(vy)^{2v-5}
\]
Proof. Let \( y > 0 \) and \( S \) is increasing in \( y \). By chain-rule, it follows that Lemma 2.7.

We believe that the bounds in Proposition 2.6 almost certainly can be improved in general. In particular, we will show that for certain designs \( y_0 = 1 \) we will need the following lemma. Before stating it, we would like to note that we found reading [Ste09] very helpful in developing its proof and we use similar ideas.

**Lemma 2.7.** Let \( \mathcal{M} = \{ z = (z_1, \ldots, z_{v-1}) \in \mathbb{R}^{v-1} | z_1 \geq z_2 \geq \ldots \geq z_{v-1} > 0 \}. \) For fixed \( y > 0 \), the function of \( (S_1(z), \ldots, S_{v-1}(z)) \) given by

\[
A_y : \{ (S_1(z), \ldots, S_{v-1}(z)) | z \in \mathcal{M} \} \rightarrow \mathbb{R},
\]

\[
(S_1(z), \ldots, S_{v-1}(z)) \mapsto \frac{(v-1) \sum_{j=0}^{v-1} (vy)^{v-1-j} S_j(z)}{\sum_{j=0}^{v-1} (vy)^{v-1-j}}
\]

is increasing in \( S_j(z), j = \{1, \ldots, v-1\} \).

**Proof.** Let \( i \in I = \{1, \ldots, v-1\} \) and \( z \in \mathcal{M} \). Then

\[
\frac{\delta S_j(z)}{\delta z_i} = \sum_{i \in J \subseteq I} \prod_{k \in J \backslash \{i\}} z_k > 0
\]

and

\[
\frac{\delta A_y(z)}{\delta z_i} = \frac{v-1}{(vy+z_i)^2 \left( \sum_{i=1}^{v-1} \frac{1}{vy+z_i} \right)^2} > 0.
\]

By chain-rule, it follows that

\[
\frac{\delta A_y((S_1(z), \ldots, S_{v-1}(z)))}{\delta S_j(z)} = \sum_{i=1}^{v-1} \frac{\delta A_y(z)}{\delta z_i} \frac{\delta z_i}{\delta S_j(z)} = \sum_{i=1}^{v-1} \frac{\delta A_y(z)}{\delta z_i} \frac{\delta z_i}{\delta S_j(z)} > 0.
\]

**Theorem 2.8.** For given \( v, b, k \), if designs with Laplacian matrix \( L[y] \) where \( L \in \mathcal{L}_{v-1}(v, b, k) \) exist for some \( y > 0 \), then they are A- and D-optimal among all designs with Laplacian matrices \( L'[y] \) with \( L' \in \mathcal{L}_1(v, b, k) \).

**Proof.** For the D-value this is immediately clear and for the A-value it follows from Lemma 2.7.

Note that for \( j = 1, \ldots, v-1 \), the function \( S_j \) is increasing and Schur-concave on \( \mathbb{R}^{v-1} \), and if \( j \neq 1 \), then \( S_j \) is strictly Schur-concave on \( \mathbb{R}_{>0}^{v-1} \) (for example [BB65], pp. 78). In particular, if a Schur-optimal design with Laplacian matrix \( L \in \mathcal{L}_1(v, b, k) \) exists, then \( L \in \mathcal{L}_{v-1}(v, b, k) \).

A special emphasis lies on the fact that the BIBD-extended designs in Theorem 2.8 are both A- and D-optimal. It has been conjectured that among RGDs the same design is A-optimal and D-optimal [JW82]. Theorem 2.8 proves the conjecture for a special case of BIBD-extended RGDs, however the conjecture is not true in general [Cak17].
3 A- and D-optimal BIBD-extended designs in \( \mathcal{L}_{v-1}(v, b, 2) \), \( b \in \{v - 1, v\} \)

For \( k = 2 \), every block of a binary design is represented by an edge in the concurrence graph and we will not make a distinction between the graph and the design. In this section we assume all designs to be connected.

### 3.1 The case \( b = v - 1 \)

Among connected designs, the A-optimal design is the reference design; this is a design that has one treatment occurring in every block and all other blocks contain each other treatment [Bai07]. Its concurrence graph is the star graph where one vertex is connected to every other vertex by exactly one edge and no other edges. All connected graphs on \( v \) vertices and \( v - 1 \) perform equally on the D-criterion for \( y = 0 \) [Bai07]. The path \( \text{Path}(v) \) is another graph in this class; this graph has vertices \( w_1, \ldots, w_v \) such that \( w_i \) and \( w_{i+1} \) are joined by an edge for \( i = 1, \ldots, v - 1 \). The Laplacian matrix of the path \( \text{Path}(v) \) is in \( \mathcal{L}_{v-1}(v, v - 1, 2) \) and the star graph minimizes \( S_j \) for all \( j = 1, \ldots, v - 1 \) among all connected graphs on \( v \) vertices with \( v - 1 \) edges [ZG08]. This proves the following proposition.

**Proposition 3.1.** Any design with Laplacian matrix \( L(\text{Path}(v))[y] \) is D-optimal (A-optimal) for and \( y \geq 0 \) \((y \geq 1)\) among connected designs with Laplacian matrix \( L[y] \) with \( L \in \mathcal{L}_1(v, v - 1, 2) \).

### 3.2 The case \( b = v \)

The cycle \( \text{Cycle}(v) \) on \( v \) vertices is a path with vertices \( w_1, \ldots, w_v, w_{v+1} = w_1 \). Bailey showed, that \( \text{Cycle}(v) \) is the adjacency graph of a connected \( D \)-optimal design and a connected A-optimal design only for \( v \leq 8 \) and \( v = 12 \) [Bai07]. For \( 9 \leq v \leq 11 \), the quadrangle of which one vertex is joined to all the remaining \( v - 4 \) vertices is A-optimal. For \( v \geq 13 \) the triangle of which one vertex is joined to the remaining \( v - 3 \) vertices is A-optimal; we will denote this graph by \( C_3(v - 3) \). For \( v = 12 \), both \( \text{Cycle}(12) \) and \( C_3(9) \) give A-optimal binary designs. It is interesting to note that \( C_3(v - 3) \) minimizes \( S_j \) for all \( j = 2, \ldots, v - 1 \) among all simple connected graphs with \( v \) edges, and further \( \text{Cycle}(v) \) maximizes \( S_j \) for all \( j = 2, \ldots, v - 1 \) among all simple connected graphs with \( v \) edges [SI09]. Since all designs in the class with Laplacian matrix in \( \mathcal{L}_2(v, v, 2) \) have a simple concurrence graph, it follows that \( L(\text{Cycle}(v)) \in \mathcal{L}_{v-1}(v, v, 2) \). This proves the following proposition.

**Proposition 3.2.** Any design with Laplacian matrix \( L(\text{Cycle}(v))[y] \) is D-optimal (A-optimal) for any \( y \geq 0 \) \((y \geq 1)\) among connected designs with Laplacian matrix \( L[y] \) with \( L \in \mathcal{L}_1(v, v, 2) \).
4 $A$- and $D$-best BIBD-extended RGDs

From now on we assume that $bk/v = r \in \mathbb{N}$, i.e. $\mathcal{L}_2(v, b, k)$ is the set of Laplacian matrices of any existing RGDs. Let $d$ be an RGD with Laplacian matrix $L_d \in \mathcal{L}_2(v, b, k)$ with $\lambda = [r(k-1)/(v-1)]$, and $d$ be a BIBD on $v$ treatments and $b$ blocks of size $k$ with Laplacian matrix $L_d$ and concurrence parameter $\lambda$. Further, let $x = \lambda + y\lambda$. We can write the Laplacian matrix $L_d + yL_d$ of the BIBD-extended RGD as

$$L[x, T_d] = (\delta + vx)I_v - T_d - xJ_v, \quad \delta = r(k-1) - \lambda(v-1).$$

The matrix $T_d$ is the adjacency matrix of a regular, simple graph $\mathcal{G}_d$. Let $\psi_1^\mathcal{G}_d \geq \psi_2^\mathcal{G}_d \geq \ldots \geq \psi_\lambda^\mathcal{G}_d$ denote the eigenvalues of $L(\mathcal{G}_d) = \delta I_v - T_d$. Then, $\psi_1^\mathcal{G}_d = 0$ since $\mathcal{G}_d$ has row sum $\delta$. The non-trivial eigenvalues of $L[x, \mathcal{G}_d]$ are $vx + \psi_1^\mathcal{G}_d, \ldots, vx + \psi_\lambda^\mathcal{G}_d$. As before, we can express the $A$- and $D$-value as a rational function and polynomial in $y$, respectively:

$$A(x, \mathcal{G}_d) = \frac{(v-1)\sum_{j=0}^{v-1}(vy)^{v-1-j}S_j(\psi_1^\mathcal{G}_d)}{\sum_{j=0}^{v-2}(vy)^{v-2-j}(v-1-j)S_j(\psi_1^\mathcal{G}_d)}$$

(4.1)

$$D(x, \mathcal{G}_d) = \sum_{j=0}^{v-1}(vy)^{v-1-j}S_j(\psi_1^\mathcal{G}_d).$$

(4.2)

**Proposition 4.1.** Let $\delta = r(k-1) - \lambda(v-1)$ and suppose, $\mathcal{L}_2(v, b, k) \neq \mathcal{L}_3(v, b, k)$.

1. For given $v, b, k$ and $x_0 = \frac{1}{v}\left((2\delta)^{v-1}\left(\frac{v-1}{v-3}\right) + 1\right)$, if there exist designs with Laplacian matrix $L[x]$ with $L \in \mathcal{L}_3(v, b, k)$ for $x \geq x_0$, then they are $D$-optimal among all designs with Laplacian matrix $L'[x]$ with $L' \in \mathcal{L}_2(v, b, k)$.

2. For given $v, b, k$ and $x_0 = (2\delta)^{v-1}\left(\frac{v-1}{v-3}\right)^2(v-3) + \frac{1}{v}$, if there exist designs with Laplacian matrix $L[x]$ with $L \in \mathcal{L}_3(v, b, k)$ for $x \geq x_0$, then they are $A$-optimal among all designs with Laplacian matrix $L'[x]$ with $L' \in \mathcal{L}_2(v, b, k)$.

**Proof.** Let $L \in \mathcal{L}_2(v, b, k)$, $L = L[x, T_d]$ where $T_d = A\mathcal{G}_d$ such that $S_3(\psi_1^\mathcal{G}_d) \geq S_3(\psi_1^{\mathcal{G}'})$ for any $\delta$-regular simple graph $\mathcal{G}'$ on $v$ vertices.

1. The Laplacian eigenvalues of a (not necessarily connected) $\delta$-regular graph are bounded from above by $2\delta$ [DB05] and with Lemma 2.3

$$|S_j(\psi_1^\mathcal{G}_d) - S_j(\psi_1^{\mathcal{G}'})| \leq \binom{v-1}{j} (2\delta)^j \leq (2\delta)^{v-1} \left(\frac{v-1}{\frac{v-1}{2}}\right), \quad j = 4, \ldots, v-1.$$

It follows for $x \geq \frac{1}{v}\left((2\delta)^{v-1}\left(\frac{v-1}{v-3}\right) + 1\right)$ that

$$\sum_{j=4}^{v-1} v^{v-1-j} x^{v-1-j} |S_j(\psi_1^\mathcal{G}_d) - S_j(\psi_1^{\mathcal{G}'})| \leq (2\delta)^{v-1} \left(\frac{v-1}{\frac{v-1}{2}}\right) \frac{(vx)^{v-4} - 1}{vx - 1}$$
2. Similarly, with Lemma 2.5 we have

\[
|S_j(\psi G_d)S_{i-j}(\psi G') - S_j(\psi G')S_{i-j}(\psi G_d)| \leq (2\delta)^i \left(\frac{v-1}{m}\right)^2, \ j = 4, \ldots, v-1.
\]

It follows for \( x \geq (2\delta)^{-1} \left(\frac{v-1}{m}\right)^2 (v-3) + \frac{1}{2} \) that

\[
\sum_{i=4}^{v-1} (vx)^{2v-3-i} \sum_{j=0}^i (v-1-j)|S_j(\psi G_d)S_{i-j}(\psi G') - S_j(\psi G')S_{i-j}(\psi G_d)|
\]

\[
\leq (2\delta)^{-1} \left(\frac{v-1}{m}\right)^2 \sum_{i=4}^{v-1} (vx)^{2v-3-i} \sum_{j=0}^i (v-1-j)
\]

\[
= (2\delta)^{-1} \left(\frac{v-1}{m}\right)^2 \sum_{i=4}^{v-1} (vx)^{2v-3-i} (i+1) \frac{2(v-1) - i}{2}
\]

\[
< (2\delta)^{-1} \left(\frac{v-1}{m}\right)^2 v(v-3)(vx)^{v-2} \sum_{i=0}^{v-5} (vx)^i
\]

\[
\leq (vx-1)(vx)^{v-2} \frac{(vx)^{v-4} - 1}{vx-1}
\]

\[
< (vx)^{2v-6}
\]

\[
\leq 3v^{2v-6} x^{2v-6} \left[S_3(\psi G_d) - S_3(\psi G')\right].
\]

The bounds in Proposition 4.1 almost certainly can be improved; computational results in our previous work showed \( x_0 = \delta + 1 \) in all considered cases Cak17.

The RGD \( d \) is fully characterized by the graph \( G_d \). We therefore want to characterize the simple regular graphs \( G \) on \( v \) vertices that give rise to \( A- \) and \( D- \) best RGDs for large \( x \) in terms of the eigenvalues of \( L(G_d) \). We will need the following definition: the complement \( \bar{G} \) of a graph \( G \) is the graph defined by the adjacency matrix \( J_v - I_v - A_G \), where \( A_G \) is the adjacency matrix of \( G \). The following proposition relates the \( A- \) and \( D- \) values given as in Equations (4.1) and (4.2) of with the complement \( \bar{G} \) of \( G \).

**Proposition 4.2.** Let \( G \) be a simple (not necessarily connected) graph and \( \bar{G} \) its complement. Then

\[
S_j(\psi \bar{G}) = \sum_{k=0}^{j} \binom{v-k-1}{j-k} (-1)^k v^{j-k} S_k(\psi G).
\]
Proof. The non-trivial Laplacian eigenvalues of the complement $\overline{G}$ are $v - \psi^G_i$ for $i = 1, \ldots, v - 1$.

Therefore

$$S_j(\psi^G) = \sum_{\mathcal{J} \subseteq \mathcal{I}, |\mathcal{J}| = j} \prod_{i \in \mathcal{J}} (v - \psi^G_i)$$

$$= \sum_{k=0}^{j} (-1)^k v^{j-k} \sum_{\mathcal{J} \subseteq \mathcal{I}} \sum_{\mathcal{K} \subseteq \mathcal{J}, i \in \mathcal{K}} |\mathcal{J}| \prod_{i \in \mathcal{K}} \psi^G_i.$$ 

In the last sum, the elementary symmetric polynomial $S_k(\psi^G)$ occurs as often as the number of ways of choosing $j$ elements with a fixed subset of $k$ from a set of $v - 1$ elements, that is $(v-k-1)$. Hence,

$$\sum_{\mathcal{J} \subseteq \mathcal{I}} \prod_{i \in \mathcal{J}} \psi^G_i = \binom{v-k-1}{j-k} S_k(\psi^G)$$

and the statement follows. \qed

Lemma 4.3. Let $G$ and $G'$ be simple $\delta$-regular graphs on $v$ vertices. Then

$$S_3(\psi^G) - S_3(\psi^{G'}) = \frac{2}{3} (\eta(G) - \eta(G')),$$

where $\eta$ is the number of $V$-subgraphs of $G$ and $G'$, that is three vertices with exactly two edges.

Proof. Since $G$ and $G'$ are $\delta$-regular, $S_1(\psi^G) = S_1(\psi^{G'})$ and $\sum_{j=1}^{v-1} (\psi^G_j)^2 = \sum_{j=1}^{v-1} (\psi^{G'}_j)^2$. With $jS_j(z) = \sum_{i=1}^{j} (-1)^{i-1} S_{j-i}(z) \sum_{i=1}^{v-1} z_i^i$ for $z \in \mathbb{R}^{v-1}$ [Mac95], it follows that

$$2S_2(\psi^G) = S_1(\psi^G)^2 - \sum_{j=1}^{v-1} (\psi^G_j)^2$$

$$3S_3(\psi^G) = \sum_{i=1}^{3} (-1)^{i-1} S_{3-i}(\psi^G) \sum_{j=1}^{v-1} (\psi^G_j)^i$$

$$= S_2(\psi^G)S_1(\psi^G) - S_1(\psi^G) \sum_{j=1}^{v-1} (\psi^G_j)^2 + \sum_{j=1}^{v-1} (\psi^G_j)^3.$$

and therefore $S_2(\psi^G) = S_2(\psi^{G'})$. The statement follows directly with

$$\sum_{j=1}^{v-1} (\psi^G_j)^2 = v\delta(\delta + 1)$$
and
\[
\sum_{i=1}^{v-1} (\psi_i^G)^3 = v\delta(\delta + 1)^2 + 2\eta(G),
\]
where \(\eta(G)\) is the number of V-subgraphs of \(G\) ([PR02] proved this equation for connected graphs but the argument directly extends to non-connected graphs).

**Theorem 4.4.** Suppose, \(\mathcal{L}_2(v,b,k) \neq \mathcal{L}_3(v,b,k)\). For given \(v, b, k\), there exists an \(x_0 > 0\) such that, if there exist designs with Laplacian matrix \(L[x]\) with \(L \in \mathcal{L}_2(v,b,k)\) for \(x \geq x_0\), then the ones whose underlying graph minimizes the number of V-subgraphs in its complement are A- and D-optimal among all designs with Laplacian matrix \(L'[x]\) with \(L' \in \mathcal{L}_2(v,b,k)\).

**Proof.** This follows directly from Lemma 4.3 and the fact that \(\rho_i = v\lambda + \psi_i\) for \(i = 1, \ldots, v-1\) and that \(S_j(z)\) are increasing in \(z\) for \(j = 1, \ldots, v-1\). 

Let \(K_{\alpha, \ldots, \alpha}\) denote the regular complete \(m\)-partite graph, that is a graph whose vertex set can be partitioned into \(m\) groups of size \(\alpha\) such that any pair of vertices is joined by an edge if and only if they are in different groups. An RGD with a multipartite concurrence graph and block size 2 is a group divisible design. [Che81] proved that regular complete bipartite graphs are the concurrence graphs of the unique A- and D-optimal designs for all \(y \geq 0\) (not necessarily only among RGDs) and extended his result to complete regular multipartite graphs for \(y = 0\). The following corollary extends the latter result to the BIBD-extension of the complete regular multipartite graph with a large number of blocks.

**Corollary 4.5.** There exists an \(x_0 > 0\) such that if there exists a design with Laplacian matrix \(L[x]\) where \(L = L(K_{\alpha, \ldots, \alpha}) \in \mathcal{L}_2(\alpha m, b, k)\) and \(x \geq x_0\), then it is A- and D-optimal among all designs with Laplacian matrix \(L'[x]\) with \(L' \in \mathcal{L}_2(\alpha m, b, k)\).

**Proof.** Follows directly from Theorem 4.4 and the fact that the complement is a union of cliques and as such V-subgraph-free. 

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