OPTIMAL DESIGNS FOR DISCRETE CHOICE MODELS VIA GRAPH LAPLACIANS

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Abstract. In discrete choice experiments, the information matrix depends on the model parameters. Therefore, $D$-optimal designs are only locally optimal in the parameter space. This dependence renders the optimization problem very difficult, as standard theory encodes $D$-optimality in systems of highly nonlinear equations and inequalities. In this work, we connect design theory for discrete choice experiments with Laplacian matrices of connected graphs. We rewrite the $D$-optimality criterion in terms of Laplacians via Kirchhoff’s matrix tree theorem, and show that its dual has a simple description via the Cayley–Menger determinant of the Farris transform of the Laplacian matrix. This results in a drastic reduction of complexity and allows us to implement a gradient descent algorithm to find locally $D$-optimal designs. For the subclass of Bradley–Terry paired comparison models, we find a direct link to maximum likelihood estimation for Laplacian-constrained Gaussian graphical models. This implies that every locally $D$-optimal design is a rational function in the parameter when the design is supported on a chordal graph. Finally, we study the performance of our algorithm and demonstrate its application on real and simulated data.

1. Introduction

Since their Nobel-laureated introduction by McFadden (1974), discrete choice experiments have enjoyed tremendous success in many applications, for example economics, psychology, public health or transportation. In this paper we consider discrete choice models with $m$ unstructured alternatives, i.e., the alternatives are considered as $m$ categories of a single factor like in a univariate one-way layout. A choice set of size $k$ is a collection of $k$ out of $m$ mutually different alternatives which corresponds to blocks in a one-way layout. We assume that each alternative from a choice set has a (latent) random utility. The consumer then decides in favor of that alternative which has the highest utility within a choice set. Hence, in contrast to the standard situation of a one-way layout, the utilities cannot be observed directly, but only which alternative has the highest utility within a choice set. This results in choice probabilities which depend on the mean utilities. Thereby the model can be reformulated as a multinomial regression model. The model with $k = 2$ alternatives per choice set is known as the Bradley–Terry paired comparison model (Bradley and Terry, 1952), which had already been introduced by Zermelo (1929) to estimate the playing strength of chess players in tournaments.

The quality of the outcome of a discrete choice experiment strongly depends on the assignment of the alternatives among different choice sets, that is the experimental design. In this paper our interest is in $D$-optimal designs for such models, that is designs which maximize the determinant of the information matrix of the experiment. Due to the inherent nonlinearity of multinomial regression, $D$-optimal designs are only locally optimal with respect to the parameter of the model. This parameter dependence makes the optimization problem much more complicated, for example in comparison with optimal designs for linear models. As a consequence, previous research is limited to restricted models.
For example, Graßhoff and Schwabe (2008) and Kahle et al. (2021) study optimal designs for the Bradley–Terry paired comparison model for \( m \in \{3, 4\} \), and describe the geometry of saturated designs, that is designs with minimal support.

In this paper, we connect design theory for discrete choice experiments with Laplacian matrices and Laplacian-constrained Gaussian graphical models. The Laplacian matrix of a weighted graph is the difference of a diagonal degree matrix and the edge weight matrix (see Section 2 for the formal definition). A Laplacian-constrained Gaussian graphical model is defined as a multivariate Gaussian with a Laplacian matrix as inverse covariance. These models are an active research area in machine learning, see e.g. Egilmez et al. (2017), Kumar et al. (2019) or Ying et al. (2021), and multivariate extremes (Röttger et al., 2021). Laplacian matrices are very relevant in combinatorics and graph theory and connect geometric, graphical and algebraic properties, see for example Devriendt (2022) for a concise introduction.

The relevance of Laplacian matrices for this work is in a reformulation of the \( D \)-optimality criterion via Kirchhoff’s matrix tree theorem. This connects Laplacian matrices and \( D \)-optimality. Each Laplacian matrix is one-to-one with a variogram or Euclidean distance matrix \( \Gamma \). Our main result is a simple dual description of the \( D \)-criterion as maximizing the logarithmic Cayley–Menger determinant

\[
\arg \max_{\Gamma} \log \det \begin{pmatrix} 0 & -\frac{1}{\Gamma}^T \\ \frac{1}{\Gamma} & -\frac{1}{\Gamma^2} \end{pmatrix} \quad \text{subject to } A\vec{\Gamma} \leq (m-1)1
\]

under simple linear inequality constraints defined by a parameter-dependent \( \binom{m}{k} \times \binom{m}{2} \) matrix \( A \). See Proposition 7 and Theorem 8 for details and notation. This simplifies the \( D \)-criterion for two reasons:

1. While the original optimization problem is defined via \( \binom{m}{k} \) variables, the dual problem is written in \( \binom{m}{2} \) variables. This results in a drastic complexity reduction for \( k > 2 \).

2. The inequalities \( A\vec{\Gamma} \leq (m-1)1 \) are sparse. Each inequality has \( \binom{k}{2} \) terms and thus the system allow for efficient algorithmic handling.

Both points are very relevant for high-dimensional problems, and allow for simple algorithms to find \( D \)-optimal designs.

Maximization of the Cayley–Menger determinant (1) under simple linear constraints appears in maximum likelihood estimation for Laplacian-constrained Gaussian graphical models (Röttger et al., 2021, Prop. 6.2). In fact, we show that for the Bradley–Terry paired comparison model \( (k = 2) \), the linear inequality constraints in Proposition 7 allow a reformulation so that the design problem is directly equivalent to Proposition 6.2 in Röttger et al. (2021), see Corollaries 11 and 12. The optimization problem (1) also has appealing properties for high-dimensional settings, as the MLE of Laplacian-constrained Gaussian graphical models exists for sample size 1 (Ying et al., 2021). The link between Bradley–Terry paired comparison models and Laplacian-constrained Gaussian graphical models further provides symbolic solutions for \( D \)-optimal design in the parameter space when the underlying graph is decomposable (Theorem 13). This follows because the maximum likelihood estimator of decomposable Laplacian-constrained Gaussian graphical model has a rational description as a matrix completion problem. Simulations indicate that every \( D \)-optimal design corresponds to a decomposable graph, see Conjecture 14. We illustrate Theorem 13 with examples in Appendix A.

In Section 5 we discuss a gradient descent algorithm and study its performance. We observe in simulations that the algorithm finds the solution of (1) very quickly and with good precision. We further apply our algorithm to two data sets from the package hyper2 (Hankin, 2017) and simulated data in Section 6. Our new methodology allows us to quickly compute a \( D \)-optimal design with respect to the estimated parameter and to evaluate the \( D \)-efficiency of the study designs. We find that in both real data sets, the study designs have a lower \( D \)-efficiency than the complete design with constant design weights. Furthermore, we observe that given the comparably similar choice
probabilities, both the study designs and the complete designs with constant design weights exhibit a measurable decrease in \( D \)-efficiency. In a simulation study, we sample parameters from a log-normal distribution for growing standard deviation. It shows that for growing standard deviation, on average both the \( D \)-efficiency of the complete design with constant weights and the support size of the \( D \)-optimal design decrease. Finally, we study the \( D \)-efficiency of the complete design with constant design weights and two complementary balanced incomplete block designs on a line in parameter space. All \texttt{R} and \texttt{Mathematica} code for the simulations, applications as well as intricate matrix operations is available as a GitHub repository

https://github.com/frank-unige/discrete_choice_designs_via_graph_Laplacians.

2. Preliminaries

2.1. Model. We study discrete choice models for \( m \) unstructured alternatives. A choice set \( C_j \subset [m] := \{1, \ldots, m\} \) is a subset of alternatives. There are \( \binom{m}{k} \) different choice sets with exactly \( k \) alternatives, such that \( j = 1, \ldots, \binom{m}{k} \). For each choice set \( C_j \), let \( Y(C_j) \) be a \( k \)-variate random vector consisting of binary components \( Y(i, C_j) \) for \( i \in C_j \). Here, \( Y(i, C_j) = 1 \) means that \( i \) is the preferred alternative in choice set \( C_j \) and \( Y(i, C_j) = 0 \) that this is not the case. For each \( i \), we have a parameter \( \pi_i > 0 \), \( i \in [m] \), the inherent, latent attractiveness (mean utility) of alternative \( i \). The model is specified by

\[
\Pr(Y(i, C_j) = 1) = \frac{\pi_i}{\sum_{s \in C_j} \pi_s}.
\]

For \( k = 2 \) one has only paired comparisons and this is the Bradley–Terry model, see e.g. Kahle et al. (2021) and Section 4. The vector \( Y(C_j) = (Y(i, C_j))_{i \in C_j} \) has a multinomial distribution with success probabilities (2). The parameters \( \pi \) are not identifiable, as multiplying the vector \( \pi \) with a scalar factor does not change the probabilities in (2). Therefore, a standard approach is to reduce the model to \( m - 1 \) parameters, for example by fixing \( \pi_m \). As this renders the remaining parameters identifiable, such a reduction is called an identifiability condition. We discuss this in detail in Section 2.5.

After a logarithmic transformation \( \beta_i = \log(\pi_i) \), the probability (2) becomes

\[
\Pr(Y(i, C_j) = 1) = \frac{\exp(\beta_i)}{\sum_{s \in C_j} \exp(\beta_s)}.
\]

This transformation allows for a reformulation as a generalized linear model, where the mean response \( \mathbb{E}(Y(i, C_j)) \) is linked to the linear predictor \( f(x_i)^T \beta = \beta_i \) with parameter vector \( \beta \in \mathbb{R}^m \) and regression vectors \( f: [m] \to \mathbb{R}^m \), \( f(x_i) = e_i \), where \( e_i \) denotes the \( i \)-th canonical unit vector, by a logit transformation. Hence, we have a multinomial regression model

\[
\Pr(Y(i, C_j) = 1) = \eta_i \left( (f(s)^T \beta)_{s \in C_j} \right).
\]

with the canonical mean response function \( \eta_i((z_s)_{s \in C_j}) = \exp(z_i) / \sum_{s \in C_j} \exp(z_s) \).

2.2. Graph Laplacians and the Farris transform. We give a short introduction to graph Laplacians and the Farris transform. For an extensive treatment, see e.g. Devriendt (2022) or Appendix A in Röttger et al. (2021).

Let \( G = (V, E) \) be a simple undirected graph with vertex set \( V = \{1, \ldots, m\} \) and edge set \( E \subseteq V \times V \). Let \( W_{uv} \) denote positive edge weights on \( G \), associated with each edge \( uv \in E \). We say that non-edges have weight 0. The Laplacian matrix \( L \) of a weighted graph is defined as follows:

\[
L_{uv} = \begin{cases} -W_{uv}, & u \neq v \\ \sum_{\ell \in \text{adj}(u)} W_{u\ell}, & u = v, \end{cases}
\]
where \( \text{adj}(u) \) denotes the set of vertices adjacent to \( u \). Therefore, the matrix \( L \) is a symmetric \( Z \)-matrix (i.e. a symmetric matrix with non-positive non-diagonal entries) with row sums equal to 0.

**Example 1.** Given the weighted graph in Figure 1 with positive edge weights \( W_{uv} \), \( uv \in E \). The Laplacian matrix of this graph equals

\[
L = \begin{pmatrix}
W_{12} + W_{13} & -W_{12} & -W_{13} & 0 \\
-W_{12} & W_{12} + W_{24} & 0 & -W_{24} \\
-W_{13} & 0 & W_{13} + W_{34} & -W_{34} \\
0 & -W_{24} & -W_{34} & W_{24} + W_{34}
\end{pmatrix}.
\]

Note that \( L1 = 0 \), i.e. that the row- and column-sums vanish.

**Remark 2.** For unweighted graphs, the combinatorial Laplacian matrix is the difference of the diagonal degree matrix \( D \) where \( D_{uv} = \lvert \text{adj}(u) \rvert \) and the adjacency matrix. This is equivalent to \( W_{uv} = 1 \) for all \( uv \in E \) in the definition above.

Let \( S_{m-1} \) be the set of symmetric \((m-1)\times(m-1)\)-matrices. The Farris transform of a matrix \( A \in S_{m-1} \) is a linear transformation resulting in the \( m \times m \) matrix \( \Gamma \) with entries

\[
\Gamma_{uv} = A_{uu} + A_{vv} - 2A_{uv}, \quad u,v < m, \\
\Gamma_{um} = \Gamma_{mu} = A_{uu}, \quad u < m, v = m, \\
\Gamma_{mm} = 0, \quad u = v = m.
\]

The matrix \( \Gamma \) lies in \( S_m^0 \), the set of symmetric \( m \times m \) matrices with zero diagonal. Furthermore, the matrix \( A \) is positive definite if and only if \( \Gamma \in C^m \), where \( C^m \subset S^m_0 \) is the cone of conditionally negative definite symmetric \( m \times m \) matrices (Engelke and Hitz, 2020; Röttger et al., 2021). The inverse Farris transform reconstructs the entries of \( A \) via

\[
A_{uv} = \frac{1}{2}(\Gamma_{um} + \Gamma_{vm} - \Gamma_{uv}).
\]

Let \( S^m_\succ \) be the cone of symmetric positive semidefinite \( m \times m \) matrices. We call \( U^m := \{ B \in S^m_\succ : B1 = 0 \} \) the set of symmetric \( m \times m \) matrices with row sums equal to zero. Let \( \Theta \in U^m \). As the diagonal entries of \( \Theta \) equal the negative of the sum of the respective non-diagonal entries in each row and column, the entries of \( \Theta \) are uniquely characterized by any \((m-1)\times(m-1)\) principal submatrix \( \Theta^{(k)} \), resulting from deleting the \( k \)-th row and column of \( \Theta \). We obtain a bijection between \( C^m \) and \( U^m \) via the Farris transform of the inverse of \( \Theta^{(k)} \).

Let \( Q_{uv} = -\Theta_{uv} \) for all \( u \neq v \) and \( Q_{uu} = 0 \) for \( 1 \leq u \leq d \). When \( Q_{uv} \geq 0 \), then \( \Theta \) is a graph Laplacian. Note that \( Q \in S^m_\succ \). The Farris transform relates to inner products as follows. Let \( \langle A, B \rangle = \text{tr}(AB) \) be the standard trace inner product on \( S^{m-1} \) and \( \langle \Gamma, Q \rangle := \sum_{s<t} \Gamma_{st}Q_{st} \) the vector...
inner product on $\mathbb{S}^m$. For arbitrary $A, \Theta^{(k)} \in \mathbb{S}^{m-1}$ and $\Gamma$ the Farris transform of $A$, it holds that
\begin{equation}
\langle A, \Theta^{(k)} \rangle = \langle \Gamma, Q \rangle.
\end{equation}

2.3. Information matrix. Let $C_j \subset V$ be a choice set of size $k$ and let $\Lambda_j(\pi)$ denote the Laplacian matrix of the complete graph $K_{C_j}$ on the vertex set $C_j$ with edge weights $\frac{\pi_{i} \pi_{s}}{\sum_{i \in C_j} \pi_{i}}$ for $s, t \in C_j$. This implies that the $k \times k$ covariance matrix of $Y(C_j)$ equals
\[
\text{Cov}(Y(C_j)) = \Lambda_j(\pi),
\]
see also Graßhoff et al. (2013). It follows that the information matrix obtained from one observation of $Y(C_j)$ computes as
\[
M(C_j, \pi) = F(C_j)\text{Cov}(Y(C_j))F(C_j)^T = F(C_j)\Lambda_j(\pi)F(C_j)^T,
\]
where $F(C_j) = (f(i))_{i \in C_j}$ denotes the $m \times k$ design matrix of $C_j$ (Graßhoff et al., 2013). Then, $M(C_j, \pi)$ is the Laplacian Matrix of the graph $(V, E(K_{C_j}))$ created from adding the nodes $V \setminus C_j$ (but no edges) to $K_{C_j}$.

2.4. Design. An experimental design for the model (2) assigns proportions of the total number of observations $N$ to the different choice sets. These proportions are called design weights. The design is encoded as a $(m)$-dimensional vector $\xi$ with non-negative entries that sum up to one. To simplify computations, one allows for the design weights to live in $\mathbb{R}$ instead of $\mathbb{N}/\mathbb{N}$. In such a case, in the spirit of Kiefer (1959, 1974), one speaks of an approximate design. We denote the set of all approximate designs for $\binom{m}{k}$ choice sets as
\[
\Delta_{(m)}^{(n)} := \{ \xi \in \mathbb{R}_{\geq 0}^{\binom{m}{k}} : \| \xi \|_1 = 1 \}.
\]
Let $\xi = (w_1, \ldots, w_{\binom{m}{k}})$ be an approximate design. Assuming independent observations, we define the information matrix of $\xi$ as the convex combination of the choice set information matrices:
\[
M(\xi, \pi) = \sum_{j=1}^{\binom{m}{k}} w_j M(C_j, \pi).
\]
If the design weights are in $\mathbb{N}/\mathbb{N}$, the matrix $N \cdot M(\xi, \pi)$ equals the classical information matrix of $N$ independent observations taken according to $\xi$. As a convex combination of graph Laplacians, the information matrix $M(\xi, \pi)$ is itself a graph Laplacian. The edge weights are $\pi_s \pi_t \sum_{j, s, t \in C_j} w_j / (\sum_{i \in C_j} \pi_i)^2$, see also Sun and Dean (2016, p. 146), thus
\begin{equation}
M_{st}(\xi, \beta) = \begin{cases} -\pi_s \pi_t \sum_{j, s, t \in C_j} \frac{w_j}{(\sum_{i \in C_j} \pi_i)^2}, & s \neq t, \\ \sum_{u \neq s} \pi_s \pi_u \sum_{j, s, u \in C_j} \frac{w_j}{(\sum_{i \in C_j} \pi_i)^2}, & s = t. \end{cases}
\end{equation}

Remark 3. A design $\xi \in \Delta_{(m)}^{(n)}$ also has a representation as a weighted $k$-uniform hypergraph $G = (V, H)$. Here, the vertices $V = [m]$ are the alternatives, and the edges $E = C_1, \ldots, C_{\binom{m}{k}}$ are the choice sets. The hyperedges are weighted with the corresponding design weights, where a zero weight determines a non-hyperedge. Then information matrices are weighted analogues of the hypergraph Laplacian matrices of Rodríguez (2009). In the Bradley–Terry model $(k = 2)$, the hypergraphs are ordinary graphs and the design defines the same undirected graph as the information matrix (Kahle et al., 2021). Small examples for $k = 2$ and $k = 3$ are shown in Figure 2.
(a) \( \binom{4}{2} = 6 \) paired comparisons

(b) \( \binom{4}{3} = 4 \) tripled comparisons

Figure 2. Complete hypergraphs for \( m = 4 \) and \( k \in \{2,3\} \)

2.5. Identifiability. Since the information matrices \( M(C_j, \pi) \) and \( M(\xi, \pi) \) are singular, the model (2) is not a-priori identifiable, but it becomes identifiable after fixing one parameter. For example, we set \( \pi_m = 1 \), such that \( \beta_m = 0 \). We write \( \pi_0 = (\pi_1/\pi_m, \ldots, \pi_{m-1}/\pi_m) \in \mathbb{R}^{m-1}_{\geq 0} \) for the parameter of the reduced model where we divide \( \pi \) by \( \pi_m \). Then \( M(\xi, \pi) = M(\xi, (\pi_0, 1)) \), as normalizing with \( \pi_m = 1 \) neither changes (2), nor the information matrix (6).

A standard approach for discrete choice models uses these identifiability constraints. For example, in Kahle et al. (2021), it is assumed that \( \pi_m = 1 \) and an \((m-1) \times (m-1)\) information matrix is computed in this reduced model. This information matrix equals \( M(m)(\xi, \pi_0) \), which is obtained from \( M(\xi, \pi) \) by deleting the \( m \)-th row and column, i.e.

\[
M_{st}^{(m)}(\xi, \pi_0) = M_{st}(\xi, \pi), \quad s, t < m.
\]

On the other hand, \( M(\xi, \pi) \) is recovered from \( M(m)(\xi, \pi_0) \) by

\[
M_{st}(\xi, \pi) = \begin{cases} 
M_{st}^{(m)}(\xi, \pi_0), & \text{for } s, t \neq m, \\
-\sum_{u=1}^{m-1} M_{su}^{(m)}(\xi, \pi_0), & \text{for } s \neq m, t = m, \\
\sum_{u=1}^{m-1} \sum_{t=1}^{m-1} M_{ut}^{(m)}(\xi, \pi_0), & \text{for } s = t = m.
\end{cases}
\]

2.6. Optimal designs. The asymptotic covariance of the maximum likelihood estimator for generalized linear models is proportional to the inverse of the information matrix (Fahrmeir and Kaufmann, 1985). This is the central reason why design theory for generalized linear models aims at maximizing the information of an experiment. Hereby, one usually chooses a function that maps the information to the real line. These functions are known as optimality criteria. But unlike in linear models, the information for generalized linear models depends on the parameter \( \pi \). This means that optimality is local in the parameter space. Among the most popular criteria is the \( D \)-criterion that maximizes the logarithmic determinant of the information:

Definition 4. Consider the criterion \( \phi: \mathbb{R}^{(m-1) \times (m-1)} \rightarrow \mathbb{R}, \phi(M) = \log \det(M) \). A design \( \xi^* \) is locally \( D \)-optimal for some parameter \( \pi_0 \) when \( \phi(M^{(m)}(\xi^*, \pi_0)) \geq \phi(M^{(m)}(\xi, \pi_0)) \) for all \( \xi \in \Delta_{m}(\pi_0) \).

Therefore, to find a locally \( D \)-optimal design for some given parameter \( \pi_0 \), we need to solve the optimization problem

\[
\xi^* = \arg\max_{\xi \in \Delta_{m}(\pi)} \phi(M^{(m)}(\xi, \pi_0)).
\]

This is an optimization problem for which both the target function and the optimization domain depend on \( \pi_0 \). The function \( \phi \) is concave and maximized over the convex set \( \Delta_{m}(\pi) \) so that this is a
convex optimization problem. Thus each local optimum (as a function of \( \xi \), not \( \pi_0 \)) is global. While each design \( \xi \in \Delta(m) \) defines a unique point in the information matrix polytope

\[
\mathcal{M} := \text{convhull}(M^{(m)}(C_j, \pi_0), 1 \leq j \leq \binom{m}{k}),
\]

the converse is not true. One could therefore also view (8) as a two-stage problem. First optimize \( \phi \) over the polytope \( \tilde{\mathcal{M}} \), yielding an optimal information matrix. This optimal matrix typically has many expressions as a convex combination of the vertices of \( \mathcal{M} \) and expressing it as such is picking an optimal design \( \xi \).

3. Optimal designs for discrete choice models

In this section we rephrase the optimization problem (8) via graph Laplacians and the Farris transform and find a simple dual of the rephrased problem. To improve readability, we simplify the notation in this section by leaving out the parameter \( \pi \), though everything is local.

By Section 2.3, the information matrix \( M(\xi) \) of a discrete choice design \( \xi = (w_1, \ldots, w_{\binom{m}{2}}) \) is the Laplacian matrix of a graph \( G \) with edge weights

\[
Q_{uv}(\xi) := \sum_{j: uv \in C_j} \frac{w_j}{\sum_{i \in C_j} \pi_i}^2.
\]

By Kirchhoff’s matrix tree theorem, we can write the determinant of the reduced information matrix in terms of the graph weights, that is

\[
\det(M^{(m)}(\xi)) = \sum_{T \in \mathcal{T}} \prod_{uv \in T} Q_{uv}(\xi),
\]

where \( \mathcal{T} \) is the set of all spanning trees of \( G \), see e.g. Röttger et al. (2021, Lemma 4.4). As a consequence, the \( D \)-criterion rewrites as

\[
\min_{\xi \in \Delta(m)} -\log \sum_{T \in \mathcal{T}} \prod_{uv \in T} Q_{uv}(\xi),
\]

subject to \( \xi \in \Delta(m) \).

We now rewrite \( Q(\xi) \) from (9) in vectorized form \( \vec{Q}(\xi) = (Q_{12}(\xi), Q_{13}(\xi), \ldots, Q_{m-1,m-1}(\xi)) \). For this, we use the lexicographic ordering \((12, 13, \ldots, (m-1)m)\) to transform a matrix from \( S_0^m \) to a \( \binom{m}{2} \)-variate vector. Similarly, let \( \vec{\Gamma}(\xi) \) denote the vectorization of \( \Gamma(\xi) \).

The following definition introduces edge-hyperedge incidence vectors and matrices which encode which edges are contained in a hyperedge, or a collection of hyperedges:

**Definition 5.** For each choice set \( C_j \) let \( s_j \) denote its incidence vector in the space of the edges of the underlying \( m \)-simplex, such that the \( uv \)-th entry of \( s_j \), where \( s_j \) is indexed in lexicographic ordering, equals

\[
s_{j,uv} = \begin{cases} 
1, & u, v \in C_j, \\
0, & \text{otherwise}.
\end{cases}
\]

Let \( S \) be the matrix whose rows are the incidence vectors, i.e. \( S^T := (s_1, \ldots, s_{\binom{m}{2}}) \). Let \( \text{supp}(\xi) = \{ C_j : w_j > 0 \} \) denote the set of choice sets with non-zero design weight. We define \( S(\xi) \) as the edge incidence matrix of all choice sets in the support of \( \xi \), so that \( S(\xi) \) is a \( |\text{supp}(\xi)| \times \binom{m}{2} \)-submatrix of \( S \) containing all incidence vectors for \( C_j \in \text{supp}(\xi) \).
Next, we define two diagonal matrices

\[ R := \text{diag}\left(\left(\sum_{i \in C_1} \pi_i\right)^2, \ldots, \left(\sum_{i \in C_{m-k}} \pi_i\right)^2\right), \]

and

\[ L := \text{diag}(\pi_1 \pi_2, \ldots, \pi_{m-1} \pi_m). \]

These matrices allow us to rewrite the vector \( \bar{Q}(\xi) \) with respect to \( \xi \) as follows:

**Lemma 6.** For a discrete choice design \( \xi \), it holds that

\[ \bar{Q}(\xi) = LS^T R^{-1} \xi. \]

Let \( \Sigma^{(m)}(\xi) \) be the inverse of the reduced information matrix \( M^{(m)}(\xi) \), and let \( \Gamma(\xi) \) be the Farris transform of \( \Sigma^{(m)}(\xi) \). The dual problem of the \( D \)-criterion (10) has a simple description in \( \Gamma(\xi) \).

**Proposition 7.** The dual problem of (10) is

(11) \[ \max_{\Gamma} \log \det \begin{pmatrix} 0 & -\frac{1}{2} \Gamma(\xi) \end{pmatrix}, \quad \text{subject to} \quad \Gamma(\xi) \in \mathbb{C}^d \text{ and } R^{-1} SL \Gamma(\xi) \leq (m - 1) 1. \]

**Proof.** Let

\[ f(\xi) = \begin{cases} -\log \sum_{T \in \mathcal{T}} \prod_{uv \in T} Q_{uv}(\xi), & \text{when } \xi \in \Delta_{(m-k)}(\xi), \\ +\infty, & \text{when } \xi \in \mathbb{R}^{(m-k)} \setminus \Delta_{(m-k)} \end{cases} \]

be an extended real-valued function, such that \( f(\xi) \) equals the objective function of (10) when \( \xi \) is a design and \( +\infty \) otherwise. Now, (10) can be reformulated as

(12) \[ \minimize_{\xi} f(\xi). \]

The Lagrangian of (10) is

\[ \mathcal{L}(\xi, B, \mu) = -\log \sum_{T \in \mathcal{T}} \prod_{uv \in T} Q_{uv}(\xi) - \langle B, \xi \rangle + \langle \mu, 1, \xi - \frac{1}{(m-k)} 1 \rangle \]

with \( B \in \mathbb{R}^{(m-k)}_+, \mu \in \mathbb{R} \). We observe that

\[ \sup_{B \geq 0, \mu} \mathcal{L}(\xi, B, \mu) = \begin{cases} -\log \sum_{T \in \mathcal{T}} \prod_{uv \in T} Q_{uv}(\xi), & \text{when } \xi \in \Delta_{(m-k)}(\xi), \\ +\infty, & \text{when } \xi \in \mathbb{R}^{(m-k)} \setminus \Delta_{(m-k)} \end{cases} \]

It follows that (12) can be rewritten as

(13) \[ \inf_{\xi} \sup_{B \geq 0, \mu} \mathcal{L}(\xi, B, \mu). \]

As all constraints in (13) are linear, duality theory (Slater’s condition) infers that (13) is invariant under swapping the infimum and supremum. The Lagrange dual function is

\[ \inf_{\xi} \mathcal{L}(\xi, B, \mu). \]
According to Röttger et al. (2021, Proposition A.5), it holds that \( \nabla Q \log \sum_{T \in T} \prod_{uv \in T} Q_{uv} = \Gamma \). It then follows from the multivariable chain rule that

\[
\frac{\partial}{\partial w_j} \left( \log \sum_{T \in T} \prod_{uv \in T} Q_{uv}(\xi) \right) = \frac{1}{(\sum_{i \in C_j} \pi_i)^2} \sum_{u \in C_j} \pi_u \pi_v \Gamma_{uv}(\xi)
\]

such that we obtain

\[
\nabla \xi \left( \log \sum_{T \in T} \prod_{uv \in T} Q_{uv}(\xi) \right) = R^{-1} SL\Gamma(\xi).
\]

The Karush-Kuhn-Tucker conditions are

\[
\begin{align*}
- R^{-1} SL\Gamma(\xi) - B + \mu \mathbf{1} &= 0, \\
\xi &\geq 0, \\
\langle \xi, \mathbf{1} \rangle &= 1, \\
\langle B, \xi \rangle &= 0, \\
B &\geq 0.
\end{align*}
\]

The first condition (14), \( B = - R^{-1} SL\Gamma(\xi) + \mu \mathbf{1} \) together with the dual feasibility \( B \geq 0 \), yields \( R^{-1} SL\Gamma(\xi) \leq \mu \mathbf{1} \). We therefore refer to all \( \Gamma(\xi) \in \mathcal{C}^d \) satisfying \( R^{-1} SL\Gamma \leq \mu \mathbf{1} \) as dually feasible points. As a consequence, evaluating the Lagrangian in the optimal point gives

\[
- \log \sum_{T \in T} \prod_{uv \in T} Q_{uv}(\xi) - \langle - R^{-1} SL\Gamma(\xi) + \mu \mathbf{1}, \xi \rangle + \langle \mu \mathbf{1}, \xi - \frac{1}{m} \mathbf{1} \rangle
\]

\[
= - \log \sum_{T \in T} \prod_{uv \in T} Q_{uv}(\xi) + \langle \Gamma(\xi), \mathbf{1} \rangle - \mu
\]

\[
= - \log \sum_{T \in T} \prod_{uv \in T} Q_{uv}(\xi) + (m - 1) - \mu.
\]

We further obtain from the fourth condition (17) that in the case of optimality

\[
\langle B, \xi \rangle = (m - 1) - \mu \langle \xi, \mathbf{1} \rangle = (m - 1) - \mu = 0,
\]

such that \( \mu = m - 1 \). This implies that the dual objective function is

\[
- \log \sum_{T \in T} \prod_{uv \in T} Q_{uv}(\xi) = - \log \det(M^{(m)}(\xi)) = \log \det(\Sigma^{(m)}(\xi)).
\]

The Cayley-Menger determinant

\[
\det(\Sigma^{(m)}(\xi)) = \det \begin{pmatrix} 0 & -1^T \\ 1 & -\Gamma(\xi) \end{pmatrix}
\]

gives the proposition. \( \square \)

In the proof of Proposition 7 we derived the Karush-Kuhn-Tucker conditions (14)-(18), which certify optimality and therefore allow an equivalent description of \( D \)-optimality:

**Theorem 8.** A discrete choice design \( \xi^* \) is \( D \)-optimal if and only if

\[
\begin{align*}
(i) \ & \xi^* \in \Delta_{\mathcal{C}^d}, \\
(ii) \ & R^{-1} SL\Gamma(\xi) \leq (m - 1) \mathbf{1}, \\
(iii) \ & \langle R^{-1} SL\Gamma(\xi) - (m - 1) \mathbf{1}, \xi \rangle = 0.
\end{align*}
\]
Note that Theorem 8 (iii) is equivalent to \((R^{-1} S L \vec{\Gamma}(\xi) - (m-1)\mathbf{1}) \cdot \xi = 0\), where \(\cdot\) denotes entry-wise multiplication.

**Example 9.** Let \(m = 6\) and \(k = 3\). The edge-hyperedge incidence matrix equals

\[
S^T = \begin{pmatrix}
1 & 2 & 3 & 4 & 5 & 6 & \vdots \\
1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\end{pmatrix}
\]

Here the choice sets \(C_1, \ldots, C_{5}\) are ordered lexicographically, starting with \(\{1, 2, 3\}\) and going to \(C_{20} = \{4, 5, 6\}\). The entries are simple indicators of the inclusion of an edge in a choice set. For example, the choice set \(C_1 = \{1, 2, 3\}\) allows for the edges \((1, 2), (1, 3), (2, 3)\), which is encoded in the first column of \(S^T\). For an arbitrary choice set \(C_j = \{s, t, u\}\), we obtain the following inequality from Theorem 8 (ii) to describe \(D\)-optimality:

\[
\frac{\pi_s \pi_t}{(\pi_s + \pi_t + \pi_u)^2} \Gamma_{st}(\xi^*) + \frac{\pi_s \pi_u}{(\pi_s + \pi_t + \pi_u)^2} \Gamma_{su}(\xi^*) + \frac{\pi_t \pi_u}{(\pi_s + \pi_t + \pi_u)^2} \Gamma_{tu}(\xi^*) \leq (m-1).
\]

By Theorem 8 (iii), equality holds in the inequality if and only if \(w_j^* = 0\). Note that the inequalities and equations are linear in \(\Gamma(\xi^*)\).

### 3.1. Kiefer–Wolfowitz theorem.

In fact, the conditions in Theorem 8 are rephrasing classical optimal design results in the Farris transform \(\Gamma\). Following Silvey (1980), the directional derivatives of \(\log \det(M^{(m)}(\xi, \pi_0))\) towards \(\log \det(M^{(m)}(C_j, \pi_0))\) are given for each \(1 \leq j \leq \binom{m}{3}\) by

\[
\langle M^{(m)}(C_j, \pi_0), M^{(m)}(\xi, \pi_0)^{-1} \rangle - (m-1).
\]

Via the Farris transform, (19) equals

\[
\langle Q(C_j, \pi), \Gamma(\xi, \pi) \rangle - (m-1),
\]

where \(Q(C_j, \pi)\) are the edge weights of the graph with Laplacian matrix \(M(C_j, \pi)\). The directional derivatives connect to \(D\)-optimality for discrete choice designs via the following application of the celebrated Kiefer–Wolfowitz equivalence theorem:

**Theorem 10** (Kiefer–Wolfowitz, see for example Silvey (1980)). A discrete choice design \(\xi^*\) is locally \(D\)-optimal in \(\pi\) if and only if

\[
\langle Q(C_j, \pi), \Gamma(\xi, \pi) \rangle \leq m - 1
\]

for all \(1 \leq j \leq \binom{m}{3}\).
According to Lemma 6, we have \(\vec{Q}(C_j, \pi) = LS^T R^{-1} e_j\), i.e. \(\vec{Q}(C_j, \pi)\) equals the \(j\)-th column of \(LS^T R^{-1}\). This means that the left hand sides of (21) are jointly expressed by
\[
(LS^T R^{-1})^T \Gamma(\xi, \pi) = R^{-1} SL \vec{\Gamma}(\xi, \pi),
\]
which shows the equivalence of (21) and Theorem 8(ii). According to Silvey (1980, Corollary 3.10), for choice sets \(C_j\) with positive weight in a locally \(D\)-optimal design \(\xi^*\), the inequalities (21) in Theorem 10 hold with equality. This is equivalent to Theorem 8(iii), while Theorem 8(i) ensures that \(\xi\) is a design.

4. Bradley–Terry paired comparison model

For the Bradley–Terry model \((k = 2)\), the edge-hyperedge incidence matrix \(S\) is the \(\binom{m}{2} \times \binom{m}{2}\) identity matrix. This leads to the following corollary of Proposition 7.

**Corollary 11.** For the Bradley–Terry paired comparison model, (11) simplifies to
\[
\text{(22) } \maximize \log \det \begin{pmatrix} 0 & -1^T \\ 1 & \Gamma(\xi) / 2 \end{pmatrix}, \text{ subject to } \Gamma(\xi) \leq \Gamma,
\]
where \(\Gamma = (m - 1)L^{-1} R 1\).

This is equivalent to the dual optimization problem for Gaussian maximum likelihood estimation under Laplacian constraints, compare for example Röttger et al. (2021) or Ying et al. (2021). In fact, Corollary 11 equals Proposition 6.2 of Röttger et al. (2021) with \(\vec{\Gamma} = (m - 1)L^{-1} R 1\) in matrix form.

We denote the choice set that contains the alternatives \(u\) and \(v\) with \((u, v)\). Let \(\lambda_{uv} := \frac{\pi_u \pi_v}{(\pi_u + \pi_v)}\).

It follows that \(\Gamma_{uv} = \frac{m - 1}{\lambda_{uv}}\). As a consequence of Corollary 11, we find the following corollary of Theorem 8:

**Corollary 12.** A Bradley–Terry design \(\xi^*\) is \(D\)-optimal if and only if
\[
\text{(i) } \xi^*_j \geq 0 \text{ for all } 1 \leq j \leq \binom{m}{2},
\]
\[
\text{(ii) } \Gamma(\xi) \leq \Gamma,
\]
\[
\text{(iii) } (\Gamma(\xi) - \Gamma) \cdot \xi = 0.
\]

The particularly simple structure of the Bradley–Terry paired comparison model allows a direct graphical interpretation of the design as graph and the design weights as edge weights. Each choice set and entry of \(\xi\) corresponds to one pair of alternatives which we always linearize in lexicographic order, i.e. \(\xi = (w_{12}, w_{13}, \ldots, w_{(m-1)m})\). Equation (9) simplifies to
\[
Q_{uv}(\xi) = \lambda_{uv} w_{uv}.
\]

Consequently, a vanishing design weight is a non-edge in the graph representation of the information matrix. Corollary 12 (iii) thus inflicts sparsity in the graph.

We now study the graphical representation of a \(D\)-optimal design for the Bradley–Terry paired comparison model in detail. A graph \(G = (V, E)\) is called decomposable when it is a complete graph or when its vertex set \(V\) can be written as a union \(V = V_1 \cup V_2\) where the induced subgraph with vertex set \(V_1 \cap V_2\) is a complete graph and the induced subgraphs with vertex sets \(V_1, V_2\) are both decomposable. A graph is decomposable if and only if it is chordal, that is all its cycles have length four or more have a chord. The following theorem illustrates how to uniquely obtain the design weights as rational functions in \(\pi\), when the support graph of the design is decomposable. In accordance with the language of graphical models, we refer to the vertex sets of complete subgraphs as cliques and to the intersection of two cliques as separators.
Theorem 13. Let $\xi^*$ be a D-optimal design for the parameter $\pi$. When the graph $G = ([m], \text{supp}(\xi^*))$ is decomposable, then $\xi^*$ is a rational function in $\pi$. Precisely, the unique D-optimal design $\xi^*$ is recovered from $\xi^*_{uv} = -\frac{M_{uv}(\xi^*, \pi)}{\lambda_{uv}}$, where we obtain $M(\xi^*, \pi)$ from $\Gamma(\xi^*, \pi)$.

Proof. When $w_{uv}^* > 0$, it is $\Gamma_{uv}(\xi^*, \pi) = \frac{w_{uv}^* - 1}{w_{uv}^*}$ according to Corollary 12 in the case of D-optimality. After reordering the alternatives according to the cliques $K_1, K_2, \ldots$ with separator sets $D_{12}, D_{13}, \ldots$, we have that each submatrix $\Gamma_{K_u \cup K_v}(\xi^*, \pi)$ is of the form

$$\Gamma_{K_u \cup K_v}(\xi^*, \pi) = \begin{pmatrix} \Gamma_{K_u \setminus K_v} & \Gamma_{K_u \setminus K_v, D_{uv}} & * \\ \Gamma_{D_{uv} \setminus K_u \setminus K_v} & \Gamma_{D_{uv}} & \Gamma_{D_{uv} \setminus K_v \setminus K_u} \\ \Gamma_{K_u \setminus K_v, D_{uv}} & \Gamma_{K_v \setminus K_u, D_{uv}} & \Gamma_{K_v \setminus K_u} \end{pmatrix},$$

with $*$ denoting the unknown entries. Hentschel (2021), showed via positive definite matrix completion (Kirkland et al., 1997, Theorem 5.3) that $\Gamma(\xi^*, \pi)$ is uniquely recovered as the conditionally negative definite completion such that $M(\xi^*, \pi)$ is the Laplacian of the underlying decomposable graph with edge weights $w_{uv}^* \lambda_{uv}$. As a consequence $\Gamma(\xi^*, \pi)$ is a rational function in $\pi$. The design weights are then obtained from $\Gamma(\xi^*, \pi)$, such that $w_{uv}^* = -\frac{M(\xi^*, \pi)_{uv}}{\lambda_{uv}}$. □

Theorem 13 only applies to decomposable graphs. Simulations indicate that generically, D-optimal designs correspond to decomposable graphs:

Conjecture 14. The graph of a D-optimal design in the Bradley–Terry model is decomposable.

In the optimization problem (22), the matrix $\Gamma$ is parameterized by the low-dimensional parameter vector $\pi \in \mathbb{R}^m$. This parameterization seems to enforce the chordality of the solution of (22), as arbitrary sample variograms $\tilde{\Gamma}$ do not necessarily imply chordality (Röttger et al., 2021). It is easy to see via Theorem 12 that (22) is equivalent to a graphical model with respect to the graph corresponding to its solution. Results from algebraic statistics for discrete graphical models (Lauritzen, 1996; Geiger et al., 2006) and Gaussian graphical models (Sturmfels and Uhler, 2010) link properties of maximum likelihood estimators with decomposable graphs. In the spirit of these results, studying the maximum likelihood degree (Huh and Sturmfels, 2014) of semidefinite Gaussian graphical models for sufficient statistics that depend on a lower dimensional parameterization could provide a proof for Conjecture 14. Solving the conjecture would also solve Kahle et al. (2021, Problem 15), as the corresponding graphs are 4-cycles and therefore non-decomposable.

We now demonstrate our new methodology for the Bradley–Terry paired comparison model via designs with complete support for three alternatives. This setting was first discussed by Graßhoff and Schwabe (2008). These designs correspond to the complete graph on three vertices. An extensive treatment of designs for four alternatives that are supported on various decomposable graphs is presented in Section A. These recover the findings of Kahle et al. (2021), but in the improved framework of the present paper. We further present an example with five alternatives in Appendix A.2. The computed symbolic solutions for the D-optimal design were unknown before, as the methods of Kahle et al. (2021) were not able to solve this problem in reasonable time. With our new methodology, the problem becomes computationally very simple, as the problem is linear in $\Gamma(\xi^*, \pi)$. The details are available in a Mathematica notebook.

Example 15. Let $m = 3$. Then, the $3 \times 3$ information matrix of a design $\xi$ equals

$$M(\xi, \pi) = \begin{pmatrix} \lambda_{12}w_{12} + \lambda_{13}w_{13} & -\lambda_{12}w_{12} & -\lambda_{13}w_{13} \\ -\lambda_{12}w_{12} & \lambda_{12}w_{12} + \lambda_{23}w_{23} & -\lambda_{23}w_{23} \\ -\lambda_{13}w_{13} & -\lambda_{23}w_{23} & \lambda_{13}w_{13} + \lambda_{23}w_{23} \end{pmatrix}.$$
By Corollary 12, a design $\xi^* = (w_{12}^*, w_{13}^*, w_{23}^*)$ with $w_{uv}^* > 0$ for all $1 \leq u < v \leq 3$ is $D$-optimal when

$$\Gamma(\xi^*, \pi) = \begin{pmatrix} 0 & \frac{2}{\lambda_{12}} & \frac{2}{\lambda_{23}} \\ \frac{2}{\lambda_{12}} & 0 & \frac{2}{\lambda_{13}} \\ \frac{2}{\lambda_{23}} & \frac{2}{\lambda_{13}} & 0 \end{pmatrix}.$$  

Via the inverse Farris transform (4), we compute

$$\Sigma^{(3)}(\xi^*, \pi_0) = \left( -\frac{1}{\lambda_{12}} + \frac{2}{\lambda_{13}} + \frac{1}{\lambda_{23}} - \frac{1}{\lambda_{12}} + \frac{1}{\lambda_{13}} + \frac{1}{\lambda_{23}} \right).$$

Inverting $\Sigma^{(3)}(\xi^*, \pi_0)$ gives the $2 \times 2$ information matrix

$$M^{(3)}(\xi^*, \pi_0) = \frac{2\lambda_{12}^2 \lambda_{13} \lambda_{23}}{\lambda_{12}^2 (\lambda_{12} - \lambda_{23})^2 - 2\lambda_{12} \lambda_{13} \lambda_{23} (\lambda_{13} + \lambda_{23}) + \lambda_{13} \lambda_{23}^2 - \lambda_{12}^2 \lambda_{13}^2 - \lambda_{13} \lambda_{23}^2},$$

We obtain from (6) that $M(\xi^*, \pi)$ is given by

$$M_{12}(\xi^*, \pi) = M^{(3)}_{12}(\xi^*, \pi_0),$$

$$M_{13}(\xi^*, \pi) = -M^{(3)}_{11}(\xi^*, \pi_0) - M^{(3)}_{12}(\xi^*, \pi_0),$$

$$M_{23}(\xi^*, \pi) = -M^{(3)}_{22}(\xi^*, \pi_0) - M^{(3)}_{12}(\xi^*, \pi_0)$$

and therefore

$$w_{12}^* = -\frac{M_{12}(\xi^*, \pi)}{\lambda_{12}} = \frac{\lambda_{13} \lambda_{23} (-\lambda_{12} \lambda_{13} - \lambda_{12} \lambda_{23} + \lambda_{13} \lambda_{23})}{\lambda_{12}^2 \lambda_{13}^2 - 2\lambda_{12} \lambda_{13} \lambda_{23} + \lambda_{13} \lambda_{23}^2 - 2\lambda_{12} \lambda_{13} \lambda_{23} + \lambda_{12}^2 \lambda_{23}^2 + \lambda_{13} \lambda_{23}^2},$$

$$w_{13}^* = -\frac{M_{13}(\xi^*, \pi)}{\lambda_{13}} = \frac{\lambda_{12} \lambda_{23} (-\lambda_{12} \lambda_{13} + \lambda_{12} \lambda_{23} - \lambda_{13} \lambda_{23})}{\lambda_{12}^2 \lambda_{13}^2 - 2\lambda_{12} \lambda_{13} \lambda_{23} + \lambda_{13} \lambda_{23}^2 - 2\lambda_{12} \lambda_{13} \lambda_{23} + \lambda_{12}^2 \lambda_{23}^2 + \lambda_{13} \lambda_{23}^2},$$

$$w_{23}^* = -\frac{M_{23}(\xi^*, \pi)}{\lambda_{23}} = \frac{\lambda_{12} \lambda_{13} (-\lambda_{12} \lambda_{13} - \lambda_{12} \lambda_{23} + \lambda_{13} \lambda_{23})}{\lambda_{12}^2 \lambda_{13}^2 - 2\lambda_{12} \lambda_{13} \lambda_{23} + \lambda_{13} \lambda_{23}^2 - 2\lambda_{12} \lambda_{13} \lambda_{23} + \lambda_{12}^2 \lambda_{23}^2 + \lambda_{13} \lambda_{23}^2}.$$

By Corollary 12, this design is $D$-optimal if and only if the design weights are non-negative. This allows to find a semi-algebraic description of the region of $D$-optimality in parameter space where a design supported on all different choice sets is $D$-optimal.

### 4.1. Saturated Designs

A saturated design is a design with minimal support with nonsingular reduced information matrix. For the Bradley–Terry paired comparison model with $m$ alternatives, saturated designs are supported on $m - 1$ design points such that the design is supported on a tree. The information matrix is the Laplacian matrix of a tree with edge weights $\lambda_{uv}$. Designs supported on trees have a particularly simple structure in the completion of $\Gamma(\xi^*, \pi)$, as it corresponds to a tree metric. This means that the missing entries compute for all $1 \leq u < v \leq m$ as

$$\Gamma_{uv}(\xi^*, \pi) = \sum_{st \in \text{ph}(u, v)} \Gamma_{st}(\xi^*, \pi),$$

where $\text{ph}(u, v)$ is the unique path between $u$ and $v$. Kahle et al. (2021) showed that $D$-optimal saturated designs always correspond to paths, i.e., trees where all nodes have degree at most two. Kahle et al. (2021) further shows that all saturated designs can be recovered via permutations of the standard path $T = 1 – 2 – 3 – \ldots – m$. For the design supported on the standard path, it follows
that $\Gamma_{uv}(\xi^*, \pi) = \frac{\lambda_{uv}}{m_{uv}}$ for $uv \in E(T) := \{12, 23, \ldots (m-1)m\}$. It follows from Kirkland et al. (1997, Cor. 2.5), that on trees it holds that

$$
\Sigma_{uv}(\xi^*, \pi) = -\sum_{uv \in \text{ph}(m, \text{lca}(u, v))} \frac{1}{M_{uv}(\xi^*, \pi)},
$$

$$
\Sigma_{uu}(\xi^*, \pi) = -\sum_{uv \in \text{ph}(m, u)} \frac{1}{M_{uv}(\xi^*, \pi)}.
$$

Here, $\text{ph}(m, \text{lca}(u, v))$ denotes the path from $m$ to the last common ancestor of $u$ and $v$ or, if $u$ is a descendant of $v$, the path from $m$ to $v$.

Now, as $\Gamma_{uv}(\xi^*, \pi) = \Sigma_{uu}(\xi^*, \pi) + \Sigma_{vv}(\xi^*, \pi) - 2\Sigma_{uv}(\xi^*, \pi)$, it holds that for $uv \in E(T)$ we have $\Gamma_{uv}(\xi^*, \pi) = -\frac{1}{M_{uv}(\xi^*, \pi)}$. Therefore for $uv \in E(T)$, we recover the well known fact that for saturated designs the nonzero design weights are all equal:

$$
w_{uv} = -\frac{M_{uv}(\xi^*, \pi)}{\lambda_{uv}} = \frac{1}{\Gamma_{uv}(\xi^*, \pi)\lambda_{uv}} = \frac{1}{m-1}.
$$

By Corollary 12, this design is $D$-optimal if and only if $\Gamma_{uv}(\xi^*, \pi) \leq \frac{m-1}{\lambda_{uv}}$ for all $uv \not\in E(T)$.

5. Algorithms

As explained in Section 4, Corollary 11 translates the optimal design problem to a Gaussian maximum likelihood estimation problem for which algorithms are available, for example those in Röttger et al. (2021); Ying et al. (2021). One such algorithm is the block descent Röttger et al. (2020) package in R. As $\Gamma$ is a dually feasible point, and every optimization step in the algorithm preserves dual feasibility, convergence is guaranteed up to the numerical precision of the employed quadratic programming solver, compare Röttger et al. (2021, p. 22). Other algorithms for this problem rely on gradient descent methods, see for example Ying et al. (2021) or Egilmez et al. (2017). For the Bradley–Terry paired comparison model it seems best to use these readily available algorithms.

For the general discrete choice problem, the linear constraint in the dual problem in Proposition 7 does not allow a simple reformulation as a coordinate-wise constraint on $\Gamma(\xi, \pi)$ like in the Bradley–Terry paired comparison model. This follows from the non-quadratic form of the edge-hyperedge incidence matrix $S$. As a consequence, the above algorithms in the previous paragraph are not applicable to solve the dual problem. Our Algorithm 1 below applies to a general discrete choice problem.

We employ the gradient descent algorithm $\text{SLSQP}$ available in the $\text{nloptr}$ package in R to find the unique optimal point $\Gamma(\xi^*, \pi)$. Again using the $\text{SLSQP}$ algorithm, we compute one $D$-optimal design $\xi^*_1$ from the optimal $\Gamma(\xi^*, \pi)$ by solving a quadratic program that minimizes $\|Q(\xi^*, \pi) - LS\Gamma(\xi^*) - L^2\|_2$ under the design constraints, where $Q(\xi^*, \pi)$ is obtained from the optimal $\Gamma(\xi^*, \pi)$.

Algorithm 1.

Input: A parameter vector $\pi \in \mathbb{R}^m_{\geq 0}$ and the choice set size $k$.

Initialize: Define the objective function $\log \det \left( \begin{smallmatrix} 0 & -1^T \\ 1 & -1 \end{smallmatrix} \right)$ and the constraint vector $R^{-1}SL\Gamma(\xi) - (m-1)1$ and their derivatives.

Computation:

1. Solve the optimization problem in $\Gamma$ using the $\text{SLSQP}$ algorithm.
2. Find a $D$-optimal design from the optimal $\Gamma^*$, again using the $\text{SLSQP}$ algorithm.

Output: A $D$-optimal design $\xi_1$, the solution $\Gamma^*$, the directional derivatives for $\xi_1$, the error in step 2.
As a potential measure of convergence, the duality gap is the difference of the primal and the dual objective functions, where we rewrite the primal problem to include the equality constraints:

\[-\log \sum_{T \in T} \prod_{uv \in T} Q_{uv}(\xi) + \langle (m-1)1, \xi - \frac{1}{\binom{m}{k}}1 \rangle - \log \det \begin{pmatrix} 0 & -1^T \\ 1 & -\Gamma(\xi) \end{pmatrix} = (m-1)(1^T \xi - 1)\].

In our computations, this function is used to assess convergence of the optimization procedure. A gap of less than $10^{-16}$ is considered as zero and the optimization problem as solved.

5.1. Performance. We study the performance of our implementation of Algorithm 1 for $m \in \{8, 10\}$ and $k \in \{3, 4, 5, 6\}$. The parameter $\pi$ is sampled uniformly from $[1, 20]^d$. Table 1 shows the largest value of the directional derivatives for the computed design, the duality gap and the computation time, averaged over $n = 10$ simulations. Note that these examples are already quite high-dimensional with respect to the design. For example for $m = 10$ and $k = 5$, there are $\binom{10}{5} = 252$ different choice sets, while $\Gamma(\xi, \pi)$ only has $\binom{10}{2} = 45$ entries. As a result for a growing number of choice sets, obtaining the optimal (and unique) $\Gamma(\xi^*, \pi)$ is much less expensive than the quadratic program that computes a $D$-optimal design from the optimal $\Gamma(\xi^*, \pi)$. The computation was conducted on a standard laptop.

| $m$ | $k$ | Dir. der. | Dual. gap | Step (1) time | Step (2) time |
|-----|-----|----------|-----------|--------------|--------------|
| 8   | 3   | 5.12e-08 | 0         | 0.05         | 0.16         |
| 8   | 4   | 3.16e-08 | 0         | 0.05         | 0.43         |
| 8   | 5   | 6.02e-08 | 0         | 0.05         | 0.19         |
| 8   | 6   | 2.21e-08 | 0         | 0.05         | 0.02         |
| 10  | 3   | 6.78e-08 | 0.18      | 2.40         | 2.40         |
| 10  | 4   | 3.74e-04 | 0.24      | 29.40        | 49.31        |
| 10  | 5   | 5.30e-05 | 0.27      | 49.31        | 21.54        |
| 10  | 6   | 1.68e-07 | 0.24      | 49.31        | 21.54        |

Table 1. The performance table shows the averaged directional derivatives, duality gaps and computation times in seconds for the two steps in Algorithm 1. We observe that finding the $D$-optimal $\Gamma$ in step (1) is fast, but deriving a $D$-optimal design from the $D$-optimal $\Gamma$ with high precision is more expensive with growing dimension.

6. Applications

In this section, we demonstrate our new methodology in applications. The $D$-efficiency of a design $\xi$ for a parameter $\pi$ is defined as

$$\text{eff}_D(\xi, \pi) = \left( \frac{\det(\Gamma(\xi^*, \pi_0))}{\det(\Gamma(\xi, \pi_0))} \right)^{\frac{1}{m-1}},$$

where $\xi^*$ is a locally $D$-optimal design for $\pi$. This means that a $D$-optimal design has $D$-efficiency one. The $D$-efficiency of a design describes the loss of information caused by a non-optimal design. For example, an efficiency of $\frac{1}{2}$ implies that twice the amount of observations is needed to obtain the same information. The computation of a $D$-optimal matrix $\Gamma(\xi^*, \pi)$ allows us to evaluate the $D$-efficiencies of specific, common discrete choice designs. As a first application, we study a poll dataset that investigates the perception of climate change.

6.1. Perception of climate change. We study the discrete choice dataset icons available in the R package hyper2 (Hankin, 2017). In the study, 124 participants from Norfolk, UK were asked to select among $k = 4$ out of $m = 6$ climate change concerns the icon that they perceive as most concerning. The icons are NB (flooding of the Norfolk Broads national park), L (London flooding due to sea level rise), PB (Polar Bear extinction), THC (slowing or stop of the thermo-haline circulation), OA
Table 2. Responses of 124 participants presented with choice sets of size 4 from a set of icons NB, L, PB, THC, OA and WAIS (see text for explanation). Each row corresponds to one choice set, such that the entries in the table correspond to the selection of each icon in the respective choice set.

| choice set | NB | L | PB | THC | OA | WAIS |
|------------|----|---|----|-----|----|------|
| 1          | 5  | 3 | 4  | 3   |    |      |
| 2          | 3  | 5 | 8  | 2   |    |      |
| 3          | 4  | 9 | 2  | 1   |    |      |
| 4          | 10 | 3 | 3  | 4   |    |      |
| 5          | 4  | 5 | 6  | 3   |    |      |
| 6          | 4  | 3 | 1  | 3   |    |      |
| 7          | 5  | 1 | 1  | 2   |    |      |
| 8          | 5  | 1 | 1  | 1   |    |      |
| 9          | 9  | 7 | 2  | 0   |    |      |

We observe that out of \( \binom{6}{2} \) possible choice sets, the study design assigns varying proportions of observations to 9 different choice sets. The \texttt{hyper2} package provides a maximum likelihood estimate

\[ \hat{\pi} = (\hat{\pi}_{\text{NB}}, \hat{\pi}_{L}, \hat{\pi}_{\text{PB}}, \hat{\pi}_{\text{THC}}, \hat{\pi}_{\text{OA}}, \hat{\pi}_{\text{WAIS}}) = (0.2523, 0.1736, 0.2246, 0.1701, 0.1107, 0.0687). \]

We compute the \( D \)-optimal approximate design for \( \hat{\pi} \) with Algorithm 1. The \( D \)-efficiencies for the study design, the complete design with constant design weights, which in this setting is the only possible balanced incomplete block design, and a rounded version (i.e. rounded such that \( w_i = \frac{n_i}{124} \) for \( n_i \in \mathbb{N}_0 \)) of the \( D \)-optimal design are as follows.

|                  | study | complete | rounded |
|------------------|-------|----------|---------|
| \( D \)-efficiency | 0.95378 | 0.96643  | 0.99997 |

We observe that the study design has the lowest efficiency.

6.2. Cricket. We study the T20 dataset available in the \texttt{hyper2} package (Hankin, 2017). It contains match results for 633 cricket matches between 13 teams in the Indian Premier League for the period from 2008 to 2017, with seven draws and three no-result matches removed. The package provides a maximum likelihood estimate \( \hat{\pi} \) for the playing strength of each team in a Bradley–Terry paired comparison model:

\[ \hat{\pi} = (0.1177, 0.0503, 0.0614, 0.0634, 0.0867, 0.0571, 0.0724, 0.1106, 0.0296, 0.0767, 0.0816, 0.0926, 0.0999) \]

The team names are available in the \texttt{hyper2} package. We compute the \( D \)-optimal design in \( \hat{\pi} \) and compute the efficiencies of the observed design and of the complete design. The results are as follows.

|                  | observed | complete |
|------------------|----------|----------|
| \( D \)-efficiency | 0.77507  | 0.98792  |

Thus the observed design has comparably low efficiency. Although the match scheduling was obviously not chosen to optimize the \( D \)-efficiency for learning the playing strength, this example demonstrates the sensitivity of the \( D \)-efficiency. Our methodology allows us to quantify the loss of \( D \)-efficiency and to certify that the complete design with constant design weights is more suitable in this setting.
6.3. Simulated parameters. We assume the setting in Example 9, i.e. let \( m = 6 \) and \( k = 3 \). We simulate parameters \( \beta_u, 1 \leq u \leq 6 \) from the centered normal distribution with varying standard deviation \( \sigma \). This implies that \( \pi_u, 1 \leq u \leq 6 \) are sampled from a log-normal distribution. We observe that \( \beta = 0 \) implies \( \pi = 1 \), i.e. the choice probabilities are all equal. In this case, it is well known that the complete design with equal design weights is \( D \)-optimal. For each of the standard deviations \( \sigma \in \{0.5, 1, 1.5, 2\} \) we simulated a parameter vector \( n = 1000 \) times and compute the \( D \)-optimal design with our implementation of Algorithm 1 and the \( D \)-efficiency of the complete design with equal weights for the simulated parameter. The averaged results are shown in Table 3. With increasing standard deviation, the sampled parameters \( \beta \) are expected to be further away from the origin, which should correspond to decreasing efficiency for the complete design with equal weights (compare also Section 6.4). Indeed, we observe this behavior in the simulation. Furthermore, the \( D \)-optimal designs have decreasing support size, which aligns well with similar observations for the Bradley–Terry paired comparison model that were discussed by Kahle et al. (2021).

| \( \sigma \)  | 0.5  | 1    | 1.5  | 2    |
|-------------|------|------|------|------|
| Directional derivatives | 5.88e-12 | 9.97e-09 | 3.34e-08 | 1.97e-05 |
| Duality gap | 0    | 1.11e-16 | 1.11e-16 | 1.08e-16 |
| \( D \)-efficiency | 0.9943 | 0.8930 | 0.6832 | 0.5414 |
| Support size | 19.9840 | 11.2850 | 6.8740 | 5.9170 |
| Time        | 0.0153 | 0.0296 | 0.0382 | 0.0473 |

Table 3. Results for logarithmic parameters sampled from a normal distribution. The table shows the average of the largest directional derivative, the duality gap, the \( D \)-efficiency of the complete design with equal weights, the support size of the \( D \)-optimal design, and the computation time of Algorithm 1. We observe decreasing efficiency of the complete design with equal design weights for increasing standard deviation of the parameter.

6.4. Efficiency comparison. In this subsection, we investigate the efficiency of the complete design with constant design weights and two balanced incomplete block designs (BIBDs) for \( m = 6 \) and \( k = 3 \). The first BIBD is defined as

\[ \xi_1^T = \frac{1}{10} (0, 1, 0, 1, 0, 1, 1, 1, 0, 0, 1, 0, 1, 0, 1, 1, 1, 0, 0, 1, 1), \]

where the individual choice sets can be recovered from the columns of the matrix \( S^T \) in Example 9. A second BIBD is defined as \( \xi_2 = \frac{1}{10} (1 - \xi_1) \). Clearly, \( \xi_1 \) and \( \xi_2 \) have complementary support.

The precise definitions of the designs are available in the R implementation. To evaluate the efficiency in a given distance from the true parameter, we compute the \( D \)-efficiency on a line in logarithmic parameter space starting in the origin. We evaluate 100 points on the line parameterized by

\[ \pi = c(\pi_1, \pi_2^{1/2}, \pi_3^{3/4}, \pi_4^{3/4}, 1), \]

where \( \pi_1 = \exp(\ell/10) \) and \( \ell = 0, 1, \ldots, 99 \). The resulting efficiencies are plotted in Figure 3. We observe that all designs are \( D \)-optimal for \( \pi = 1 \), as we would expect from design theory. As in Section 6.3, it shows that increasing Euclidean distance to the origin decreases the \( D \)-efficiency of the complete design with constant design weights. For \( \ell = 100 \), we compute the \( D \)-optimal design

\[ \xi^* \approx (0, 0, 0.19196, 0, 0.20127, 0.21450, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0.39228, 0, 0, 0, 0). \]
Figure 3. Efficiencies for 100 points on a line starting in the origin for three designs. The solid line corresponds to the complete design with constant weights, the dashed to the BIBD $\xi_1$ and the dotted line to the BIBD $\xi_2$.

We observe that the support of $\xi^*$ is contained in the support of $\xi_1$. Besides, the $D$-efficiency of the complete design with constant design weights lies between the $D$-efficiencies of $\xi_1$ and $\xi_2$ in Figure 3, further suggesting that this results from the complementary supports of the designs.

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Appendix A. Solutions for the Bradley–Terry Design Problem

In this section we discuss decomposable examples for the Bradley–Terry paired comparison model. In this case, for four alternatives (\(m = 4\)), Kahle et al. (2021) found explicit formulas, expressing the \(D\)-optimal design weights in terms of the parameters, thereby solving the optimal design problem. We first express the \(m = 4\) solutions much more efficiently in our new framework. Then in Section A.2, we give previously unknown solutions for five alternatives.

A.1. Four Alternatives. We begin with the complete graph, i.e. designs with full support.

Example 16. Let \(m = 4\). Then, the reduced information matrix \(M(\xi, \pi_0)\) of a design \(\xi\) that is supported on the complete graph computes as

\[
\begin{pmatrix}
\lambda_{12}w_{12} + \lambda_{13}w_{13} + \lambda_{14}w_{14} & -\lambda_{12}w_{12} & -\lambda_{13}w_{13} \\
-\lambda_{12}w_{12} & \lambda_{12}w_{12} + \lambda_{23}w_{23} + \lambda_{24}w_{24} & -\lambda_{23}w_{23} \\
-\lambda_{13}w_{13} & -\lambda_{23}w_{23} & \lambda_{13}w_{13} + \lambda_{23}w_{23} + \lambda_{34}w_{34}
\end{pmatrix}
\]

Now, from Corollary 12 the fully supported design \(\xi^*\) is \(D\)-optimal when

\[
\Gamma(\xi^*, \pi) = \begin{pmatrix}
0 & \frac{3}{\lambda_{12}} & \frac{3}{\lambda_{13}} & \frac{3}{\lambda_{14}} \\
\frac{3}{\lambda_{12}} & 0 & \frac{3}{\lambda_{23}} & \frac{3}{\lambda_{24}} \\
\frac{3}{\lambda_{13}} & \frac{3}{\lambda_{23}} & 0 & \frac{3}{\lambda_{34}} \\
\frac{3}{\lambda_{14}} & \frac{3}{\lambda_{24}} & \frac{3}{\lambda_{34}} & 0
\end{pmatrix}
\]

where \(\lambda_{uv} = \frac{\pi_u \pi_v}{(\pi_u + \pi_v)^2}\). Via the inverse Farris transform, we find

\[
\Sigma(\xi^*, \pi_0) = \begin{pmatrix}
\frac{3}{2} \left( -\frac{1}{\lambda_{12}} + \frac{1}{\lambda_{14}} + \frac{1}{\lambda_{24}} \right) & \frac{3}{2} \left( -\frac{1}{\lambda_{12}} + \frac{1}{\lambda_{14}} + \frac{1}{\lambda_{24}} \right) \\
\frac{3}{2} \left( -\frac{1}{\lambda_{12}} + \frac{1}{\lambda_{14}} + \frac{1}{\lambda_{24}} \right) & \frac{3}{2} \left( -\frac{1}{\lambda_{12}} + \frac{1}{\lambda_{14}} + \frac{1}{\lambda_{24}} \right)
\end{pmatrix}
\]

We compute the Information matrix \(M(\xi^*, \pi)\) from \(\Sigma(\xi^*, \pi_0)\) and display the entry in \(w_{12} = 12\):

\[
M_{12}(\xi^*, \pi) = \frac{1}{A} (-\lambda_{12}\lambda_{13}\lambda_{14}\lambda_{23}\lambda_{24} - \lambda_{12}\lambda_{13}\lambda_{14} + \lambda_{12}\lambda_{13}\lambda_{24} - \lambda_{12}\lambda_{14}\lambda_{24})
\]

with some normalization term \(A\). We obtain \(w_{12} = -\frac{M_{12}(\xi^*, \pi)}{\lambda_{12}}\). The design is \(D\)-optimal when all weights are positive, i.e. when \(\xi^* \in \Delta_6\).

Example 17. Let \(m = 4\) and assume a design \(\xi\) supported on the chordal graph in Figure 4. Then,
the reduced information matrix of such a design computes as

\[
M^{(4)}(\xi, \pi_0) = \begin{pmatrix}
\lambda_{13}w_{13} + \lambda_{14}w_{14} & 0 & 0 & -\lambda_{13}w_{13} \\
0 & \lambda_{23}w_{23} + \lambda_{24}w_{24} & -\lambda_{23}w_{23} & -\lambda_{13}w_{13} \\
-\lambda_{13}w_{13} & -\lambda_{23}w_{23} & \lambda_{13}w_{13} + \lambda_{23}w_{23} + \lambda_{34}w_{34} & 0 \\
0 & 0 & 0 & \lambda_{23}w_{23} + \lambda_{34}w_{34}
\end{pmatrix}.
\]

We obtain from Corollary 12 that

\[
\Gamma(\xi^*, \pi) = \begin{pmatrix}
0 & \Gamma_{12} & \frac{3}{\lambda_{13}} & \frac{3}{\lambda_{14}} \\
\Gamma_{12} & 0 & \frac{3}{\lambda_{23}} & \frac{3}{\lambda_{24}} \\
\frac{3}{\lambda_{13}} & \frac{3}{\lambda_{23}} & 0 & \frac{3}{\lambda_{24}} \\
\frac{3}{\lambda_{14}} & \frac{3}{\lambda_{24}} & \frac{3}{\lambda_{24}} & 0
\end{pmatrix},
\]

where \(\Gamma_{12}\) denotes the unknown entry in \(\Gamma(\xi^*, \pi)\). Via the Farris transform, we find

\[
\Sigma^{(4)}(\xi^*, \pi_0) = \begin{pmatrix}
\frac{3}{\lambda_{13}} & \sigma_{12} & \frac{3(\lambda_{13}\lambda_{14} + \lambda_{13}\lambda_{34} - \lambda_{14}\lambda_{34})}{2\lambda_{13}\lambda_{14}\lambda_{34}} \\
\sigma_{12} & \frac{3}{\lambda_{24}} & \frac{3(\lambda_{23}\lambda_{24} + \lambda_{23}\lambda_{34} - \lambda_{24}\lambda_{34})}{2\lambda_{23}\lambda_{24}\lambda_{34}} \\
\frac{3(\lambda_{13}\lambda_{14} + \lambda_{13}\lambda_{34} - \lambda_{14}\lambda_{34})}{2\lambda_{13}\lambda_{14}\lambda_{34}} & \frac{3(\lambda_{23}\lambda_{24} + \lambda_{23}\lambda_{34} - \lambda_{24}\lambda_{34})}{2\lambda_{23}\lambda_{24}\lambda_{34}} & \frac{1}{\lambda_{34}}
\end{pmatrix},
\]

where \(\sigma_{12} = \frac{1}{2}(\frac{3}{\lambda_{13}} + \frac{3}{\lambda_{24}} - \Gamma_{12})\). According to Bakonyi and Woerdeman (2011, Theorem 2.2.3), there is only one positive definite solution for \(\sigma_{12}\) such that \((\Sigma^{(4)}(\xi^*, \pi_0))^{-1}\) is \(D\)-optimal, namely

\[
\sigma_{12} = \frac{3(\lambda_{13}\lambda_{14} + \lambda_{14}\lambda_{34} - \lambda_{13}\lambda_{34})}{2\lambda_{13}\lambda_{14}\lambda_{34}} \frac{3(\lambda_{23}\lambda_{24} + \lambda_{23}\lambda_{34} - \lambda_{24}\lambda_{34})}{2\lambda_{23}\lambda_{24}\lambda_{34}} - \frac{1}{\lambda_{34}}.
\]

Via the inverse of \(\Sigma^{(4)}(\xi^*, \pi_0)\) we obtain the \(D\)-optimal information matrix \(M(\xi^*, \pi)\) where the entries are rational functions of \(\lambda_{uv}\) and hence the design weights \(w_{uv}^* = -\frac{M_{uv}(\xi^*, \pi)}{\lambda_{uv}}\). The design \(\xi^*\) is \(D\)-optimal when \(\Gamma_{12}(\xi^*, \pi) \leq \frac{3}{\lambda_{13}}\) and when \(\xi^* \in \Delta_6\).

**Example 18.** Let \(m = 4\) and assume a design \(\xi) supported on the chordal graph in Figure 5. Then,
We obtain from Corollary 12 that

$$\Gamma(\xi^*, \pi) = \begin{pmatrix}
\begin{array}{cccc}
0 & \Gamma_{12} & \Gamma_{13} & \frac{3}{\lambda_{14}} \\
\Gamma_{12} & 0 & \frac{3}{\lambda_{23}} & \frac{3}{\lambda_{24}} \\
\Gamma_{13} & \frac{3}{\lambda_{23}} & 0 & \frac{3}{\lambda_{34}} \\
\frac{3}{\lambda_{14}} & \frac{3}{\lambda_{24}} & \frac{3}{\lambda_{34}} & 0
\end{array}
\end{pmatrix},
$$

where $\Gamma_{12}, \Gamma_{13}$ denote the unknown entries of $\Gamma(\xi^*, \pi)$. Via the Farris transform we obtain

$$\Sigma^{(4)}(\xi^*, \pi_0) = \begin{pmatrix}
\begin{array}{ccc}
\frac{3}{\lambda_{14}} & \sigma_{12} & \sigma_{13} \\
\sigma_{12} & \frac{3(\lambda_{23} \lambda_{24} + \lambda_{25} \lambda_{34} - \lambda_{24} \lambda_{35})}{2\lambda_{23} \lambda_{24} \lambda_{35}} & \frac{3\lambda_{23} \lambda_{24} \lambda_{35} + \lambda_{24} \lambda_{35}}{3} \\
\sigma_{13} & \frac{3\lambda_{23} \lambda_{24} \lambda_{35} - \lambda_{24} \lambda_{35}}{2\lambda_{23} \lambda_{24} \lambda_{35}} & \frac{3\lambda_{23} \lambda_{24} \lambda_{35} + \lambda_{24} \lambda_{35}}{3}
\end{array}
\end{pmatrix},
$$

where $\sigma_{12} = \frac{1}{2}(\frac{3}{\lambda_{14}} + \frac{3}{\lambda_{24}} - \Gamma_{12})$ and $\sigma_{13} = \frac{1}{2}(\frac{3}{\lambda_{14}} + \frac{3}{\lambda_{34}} - \Gamma_{13})$. From the block structure of the information matrix we immediately obtain that the positive definite matrix completion is $\sigma_{12} = \sigma_{13} = 0$. Via the inverse of $\Sigma^{(4)}(\xi^*, \pi_0)$ we obtain the $D$-optimal information matrix $M(\xi^*, \pi)$ where the entries are rational functions of $\lambda_{uv}$ and hence the design weights $w^*_{uv} = -\frac{M_{uv}(\xi^*, \pi)}{\lambda_{uv}}$. The design $\xi^*$ is $D$-optimal when

$$\Gamma_{12}(\xi^*, \pi) = \frac{3}{\lambda_{14}} + \frac{3}{\lambda_{24}} \leq \frac{3}{\lambda_{12}}$$

and $\xi^* \in \Delta_6$.

A.2. Five alternatives. We only discuss the complete graph for the setting with five alternatives.

**Example 19.** Similarly to Example 16, we obtain from Corollary 12 that $D$-optimality of a fully-supported design holds when

$$\Gamma(\xi^*, \pi) = \begin{pmatrix}
\begin{array}{cccc}
0 & \frac{4}{\lambda_{12}} & \frac{4}{\lambda_{13}} & \frac{4}{\lambda_{14}} & \frac{4}{\lambda_{15}} \\
\frac{4}{\lambda_{12}} & 0 & \frac{4}{\lambda_{23}} & \frac{4}{\lambda_{24}} & \frac{4}{\lambda_{25}} \\
\frac{4}{\lambda_{13}} & \frac{4}{\lambda_{23}} & 0 & \frac{4}{\lambda_{34}} & \frac{4}{\lambda_{35}} \\
\frac{4}{\lambda_{14}} & \frac{4}{\lambda_{24}} & \frac{4}{\lambda_{34}} & 0 & \frac{4}{\lambda_{45}} \\
\frac{4}{\lambda_{15}} & \frac{4}{\lambda_{25}} & \frac{4}{\lambda_{35}} & \frac{4}{\lambda_{45}} & 0
\end{array}
\end{pmatrix},
$$

where $\lambda_{uv} = \frac{\pi_u \pi_v}{(\pi_u + \pi_v)^2}$. We obtain the $D$-optimal information matrix as a rational function in $\lambda_{uv}$, $1 \leq u < v \leq 5$, such that $w^*_{uv} = -\frac{M_{uv}(\xi^*, \pi)}{\lambda_{uv}}$. The design is $D$-optimal if and only if $\xi^* \in \Delta_{10}$. The full computation is available in a Mathematica notebook.

**Example 20.** Let $m = 4$ and assume a design $\xi$ supported on the chordal graph in Figure 6. Then, the reduced information matrix $M^{(5)}(\xi, \pi_0)$ computes as

$$M^{(5)}(\xi, \pi_0) = \begin{pmatrix}
\begin{array}{cccccc}
\lambda_{15}w_{15} + \lambda_{12}w_{12} & -\lambda_{12}w_{12} & 0 & 0 \\
-\lambda_{12}w_{12} & \lambda_{12}w_{12} + \lambda_{25}w_{25} & 0 & 0 \\
0 & 0 & \lambda_{34}w_{34} + \lambda_{35}w_{35} & -\lambda_{34}w_{34} \\
0 & 0 & \lambda_{34}w_{34} & \lambda_{34}w_{34} + \lambda_{45}w_{45}
\end{array}
\end{pmatrix}.$$
We obtain from Corollary 12 that

\[
\Gamma(\xi^*, \pi) = \begin{pmatrix}
0 & \frac{4}{\lambda_{12}} & \Gamma_{13} & \Gamma_{14} & \frac{4}{\lambda_{15}} \\
\frac{4}{\lambda_{12}} & 0 & \Gamma_{23} & \Gamma_{24} & \frac{1}{\lambda_{25}} \\
\Gamma_{13} & \Gamma_{23} & 0 & \frac{4}{\lambda_{34}} & \frac{1}{\lambda_{35}} \\
\Gamma_{14} & \Gamma_{24} & \frac{1}{\lambda_{34}} & 0 & \frac{4}{\lambda_{45}} \\
\frac{4}{\lambda_{15}} & \frac{4}{\lambda_{25}} & \frac{1}{\lambda_{35}} & \frac{1}{\lambda_{45}} & 0
\end{pmatrix},
\]

From the simple block structure of \(\Sigma^{(5)}(\xi^*, \pi_0)\) we obtain the D-optimal information matrix \(M(\xi^*, \pi)\) where the entries are rational functions of \(\lambda_{uv}\) and hence the design weights \(w^*_uv = \frac{M_{uv}(\xi^*, \pi)}{\lambda_{uv}}\). The design \(\xi^*\) is D-optimal when

\[
\begin{align*}
\Gamma_{13} &= \frac{4}{\lambda_{15}} + \frac{4}{\lambda_{35}} \leq \frac{4}{\lambda_{13}}, \\
\Gamma_{14} &= \frac{4}{\lambda_{15}} + \frac{4}{\lambda_{45}} \leq \frac{4}{\lambda_{14}}, \\
\Gamma_{23} &= \frac{4}{\lambda_{25}} + \frac{4}{\lambda_{35}} \leq \frac{4}{\lambda_{23}}, \\
\Gamma_{24} &= \frac{4}{\lambda_{25}} + \frac{4}{\lambda_{45}} \leq \frac{4}{\lambda_{24}}.
\end{align*}
\]