The Polyhedral Geometry of Graphical Designs

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Abstract

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A graphical design is a quadrature rule for a graph. That is, a graphical design is a subset of graph vertices for which the global averages of certain Laplacian eigenvectors are equal to weighted averages of these vectors over the design subset. This definition was inspired by classical quadrature rules on the sphere. This thesis refines and extends the initial definition of graphical designs, which was left with ambiguity, to graphs with positive edge weights.

Through Gale duality, we establish a bijection between graphical designs and the face lattices of the eigenpolytopes of a graph. This connection proves the existence of positively weighted graphical designs averaging any collection of eigenvectors of a graph, and provides methods to compute, organize, and optimize graphical designs. These tools are then applied to three families of graphs: cocktail party graphs, cycles, and cubes.

This thesis also considers complexity and algorithms for related computational questions. We show the universality of eigenpolytopes for positively weighted graphs; that is, every polytope up to affine equivalence appears as the eigenpolytope of a positively weighted graph, and we provide a strongly polynomial time algorithm for this construction. As a stepping stone, we show that given an appropriate orthogonal basis of $\mathbb{R}^n$ and a partition of these basis vectors, there is a positively weighted graph which has Laplacian eigenspaces specified by this basis and partition. These algorithms establish the first complexity results for graphical designs, piggybacking off of complexity results for polytopes.

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DEDICATION

To Ken Bube, for believing in me when no one else did. Without your support and encouragement I would not be writing a thesis today.

Chapter 1

INTRODUCTION

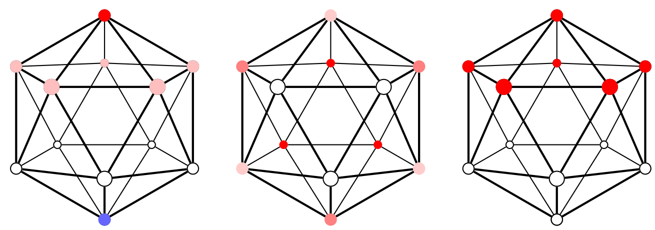
A graphical design is a quadrature rule for a graph $G = ([n], E, w)$, where $[n] := \{1, 2, \ldots, n\}$ is the set of vertices of the graph, $E \subseteq [n] \times [n]$ is the edge set, and $w : E \to \mathbb{R}_{>0}$ defines positive edge weights. Generally, a quadrature rule is a numerical method to approximate the global average of a function on a domain by sampling the function on a smaller, finite subset. Graphical designs were first defined by Steinerberger in [96] for unweighted graphs, drawing inspiration from numerical integration on the sphere. Part of my work has refined and generalized the initial definition of graphical designs to the following.

Definition 1.0.1. Let $L \in \mathbb{R}^{n \times n}$ be a symmetric operator on $G = ([n], E, w)$, which has m distinct eigenspaces arbitrarily ordered as $\Lambda_1 < \ldots < \Lambda_m$. A *$k$-graphical design* of G is a subset $S \subseteq [n]$ and real weights $(a_s \neq 0 : s \in S)$ such that for any $\varphi \in \Lambda_1, \ldots, \Lambda_k$,

$$\sum_{s \in S} a_s \varphi(s) = \frac{1}{n} \sum_{i=1}^{n} \varphi(i) \tag{1.1}$$

In [96], graphical designs were defined by averaging individual eigenvectors of $AD^{-1} - I$ in a particular ordering, and it was left open how to resolve the issue of eigenvalue multiplicity. In the continuous setting, eigenvalue multiplicity does not pose a major challenge. However, for graphs, there may be large eigenspaces at any place in the spectrum. When this is the case, it is unclear how to pick an eigenbasis or how to break ties among eigenvectors with the same eigenvalue. Averaging entire eigenspaces avoids these issues. We have also extended the scope of graphical designs to other graph operators and to arbitrary eigenspace orderings.

We consider three types of quadrature weights for graphical designs: arbitrary ($a_s \in \mathbb{R}^*$), positive ($a_s > 0$), and combinatorial ($a_s = a_{s'}$ for all $s, s' \in S$). The three types of weights are illustrated in Fig. 1.1. Negative weights are typically undesirable for numerical reasons, as they can lead to unstable or divergent solutions [51]. Combinatorial weights are very restrictive and may not always exist, hence we often focus on positive weights in this thesis. We note that there are two types of weights at play in graphical designs – the graph edge weights $(w(ij) : ij \in E)$ and the quadrature weights $(a_s : s \in S)$. We will at times refer to graphical designs simply as *designs* for brevity.



(a) (b) (c)

Figure 1.1: Three graphical designs of the icosahedral graph in a fixed eigenspace ordering. Lighter colors represent weights of smaller magnitude, red indicates positive and blue is negative. (A) shows an arbitrarily weighted 3-graphical design, (B) shows a positively weighted 3-graphical design, and (C) shows a combinatorial 2-graphical design.

Graphical designs provide a method for graph sampling. Modern data is often modeled by graphs, such as online communities, power grids, and transit networks. As our data evolves, so must our data processing tools. The relatively new field of graph signal processing [75, 76] translates traditional signal processing techniques to graphs. Graph sampling is a major challenge studied in this field – [97] is evidence that graphical designs sample effectively.

In [96], graphical designs were first defined for unweighted graphs by the *low frequency* eigenvectors of $L = AD^{-1} - I$, a normalized graph Laplacian, using arbitrary weights. The spectrum of $AD^{-1} - I$ is contained in $[-2, 0]$; high frequency eigenvectors have an eigenvalue near -1, and low frequency eigenvectors have an eigenvalue near -2 or 0. This provides a particular ordering of the eigenspaces. Exactly averaging low frequency eigenvectors mimics the construction of spherical t-designs [28], which are quadrature rules for the sphere that exactly integrate low degree polynomials. Low degree polynomials are the low frequency eigenfunctions of the Laplace-Beltrami operator on the sphere.

This thesis consists of two papers, which are each summarized in the rest of this chapter. I also summarize [5] in 1.1, which served as my master's thesis at the University of Washington. This paper investigates combinatorial designs in highly structured regular graphs, and distinguishes combinatorial graphical designs in the frequency order from related combinatorial concepts. Chapter 2 establishes a bijection between positively weighted graphical designs in regular graphs and the facial structure of certain polytopes arising from the eigenspaces of a graph, known as eigenpolytopes. Chapter 3 shows that any polytope up to affine equivalence appears as the eigenpolytope of a positively weighted graph. The proof is a constructive algorithm, and moreover strongly polynomial time. We then extend the bijection from the previous chapter to positively weighted graphs, and use these two results together to provide the first complexity results for graphical designs: it is #P-complete to count the number of support minimal graphical designs, it is NP-hard to find a minimum cardinality graphical design, and it is strongly NP-complete to determine if there is a graphical design with support smaller than a bound arising from the eigenpolytope connection.

1.1 Previous Work: Codes, Cubes, and Graphical Designs

My master's thesis [5] was published in the *Journal of Fourier Analysis and Applications* in a special issue on harmonic analysis on graphs. This paper connects combinatorial graphical designs on the cube graph to linear error correcting codes, distinguishes combinatorial graphical designs in the frequency order from several related combinatorial concepts, and resolves the issues posed by eigenspaces with multiplicity.

1.1.1 Background

This paper was primarily motivated by two observations:

1. The computed examples of graphical designs with few vertices tended to be nicely spaced out and symmetric on highly structured graphs [96, 43].

2. Graphical designs have an obvious similarity to t-designs in association schemes (see [66, Chapter 21]).

Here, we focus only on graphical designs in the frequency order, which we recall orders the eigenspaces of $AD^{-1} - I$ from the "outside in" on the interval $[-2, 0]$. We are also interested in the concept of *extremal designs* [43], which are graphical designs that average all but one eigenspace. To quantify how 'good' a graphical design is, we introduce the concept of *efficacy.*

Definition 1.1.1. If $S \subset [V]$ is a k-graphical design but not a $(k+1)$-graphical design in the frequency order, its efficacy is

$$\text{efficacy}(S) = \frac{|S|}{\sum_{i=1}^{k} \dim \Lambda_i}$$

We say a graphical design with a lower efficacy is *more effective.*

1.1.2 Results

We start by resolving the open question of [96] about how to deal with eigenspace multiplicity. In the continuous setting, there are folklore heuristics which essentially imply an eigenspace is never 'too fat' to be a problem. Thus in spherical designs or analogous sampling problems on Riemannian manifolds [95], it is sufficient to define quadrature rules in terms of individual eigenfunctions rather than entire eigenspaces. This is not true in the case of graphs, where high frequency eigenspaces may have high dimension and lead to ambiguity. Thus we reinterpret graphical designs in terms of averaging entire eigenspaces, rather than eigenvector by eigenvector, and justify this choice.

We next consider combinatorial graphical designs in the edge graphs of hypercubes. Let Q_d denote the edge graph of the d-dimensional hypercube, which has vertices $\{0, 1\}^d$ and an edge between vertices which differ on exactly one coordinate. The spectral graph theory of Q_d is well studied. For each $v \in \{0,1\}^d$, there is an eigenvector $\varphi_v \in \{\pm 1\}^{\{0,1\}^d}$ whose coordinates are given by $\varphi_v(x) = (-1)^{v^\top x}$ for $x \in \{0,1\}^d$. We show that length d linear error correcting codes provide combinatorial graphical designs on Q_d. A length d linear error correcting code C can be represented as the 0-1 kernel of a check matrix $M \in \{0,1\}^{k \times d}$; that is, $C = \{x \in \{0,1\}^d : Mx = 0\}$. We show that the eigenvectors which a linear code M averages are entirely determined by its check matrix M. Using this result, we show that the Hamming code [86] of length $2^r - 1$ is a particularly effective extremal design on Q_{2^r-1}. Moreover, we can lift the Hamming code of length $2^r - 1$ to linear codes of length 2^r and $2^r + 1$ which are also effective extremal designs on Q_{2^r} and Q_{2^r+1}, respectively. We can also project the Hamming code down one dimension with only a slight loss of these properties.

The remainder of the paper is devoted to distinguishing graphical designs in the frequency order from related combinatorial concepts. The extremal designs of [43] allow for any eigenspace ordering. We dig a little deeper into the specific extremal constructions presented in [43] and show that they are typically incompatible with the frequency ordering on the eigenspaces. The projected Hamming code from the previous section also shows that there may be non-extremal graphical designs in the frequency ordering which are highly effective. We also provide several examples of effective and/or extremal graphical designs that are not stable sets.

Lastly, we consider the notion of t-designs in association schemes (see [27, 66]). In broad strokes, a (symmetric) s-class association scheme is a highly structured coloring of the edges of the complete graph into $s + 1$ relationship classes. Taking the edges specified by any subset of the relationship classes provides a graph. The graphs Q_d and the Kneser graphs $KG(n, k)$ are examples of graphs that arise in this manner. Any graph arising from the same association scheme has eigenspaces spanned by $s + 1$ common blocks of eigenvectors, though some of these blocks may collapse together. For this summary, suppose each of these blocks remains a distinct eigenspace of some graph arising from an association scheme. An association scheme can further have the property of being *q-polynomial*, which provides a specific ordering on these eigenspaces. A t-design in a q-polynomial association scheme is a combinatorial t-graphical design in this specific q-polynomial ordering. We show, however, that this q-polynomial ordering is typically not the same as the frequency ordering. There is a more general notion of T-designs in association schemes which do not require the extra condition of being q-polynomial. These are exactly combinatorial $|T|$-graphical designs for some choice of order on the eigenspaces. At the time, we were focused on the frequency order and hence do not explicitly state this connection to T-designs.

1.2 Graphical Designs and Gale Duality

Chapter 2 is [6], which is joint work with Rekha Thomas. This paper was published in *Math Programming*. We use the theory of Gale duality to establish a bijection between positively weighted graphical designs on regular graphs and the faces of the *eigenpolytopes* associated to a graph. This bijection provides a proof of the existence of positively weighted graphical designs for every k, an upper bound on the cardinality of a positively weighted k-design, and a method to organize, compute, and optimize graphical designs. These tools are then applied to several families of Cayley graphs, including further work on the cube graphs Q_d.

1.2.1 Background

This paper was sparked by the observation that the eigenspaces of AD^{-1} for a regular graph $G = (V, E)$ provide vector configurations which are dual as oriented matroids. Further, because the nontrivial eigenvectors of AD^{-1} are orthogonal to $\mathbb{1}$, the all-ones vector, a positively weighted graphical design is really a linear dependence on one of the vector configurations arising from the graph. Here, we broaden our scope to positive quadrature weights and arbitrary orderings of the eigenspaces of AD^{-1}. We now explain some of the background and notation needed to state the results of this paper.

Let $G = (V, E)$ have m eigenspaces, and let $k \in \{2, \ldots, m-1\}$. Let U denote the matrix whose rows are the eigenvectors of AD^{-1} arranged by eigenspace. We will split this matrix into two chunks: $U_{\boldsymbol{k}}$, which consists of the rows corresponding to $\Lambda_2, \ldots, \Lambda_k$, and $U_{\bar{\boldsymbol{k}}}$, which consists of all the other rows, namely the rows corresponding to $\Lambda_1, \Lambda_{k+1}, \ldots, \Lambda_m$. Consider the vector configurations given by the columns of these submatrices and call them $\mathcal{U}_{\boldsymbol{k}}$ and $\mathcal{U}_{\bar{\boldsymbol{k}}}$ respectively. We illustrate this process in Figure 1.2. Note that the rows of $U_{\boldsymbol{k}}$ form a basis for the nullspace of $U_{\bar{\boldsymbol{k}}}$ by orthogonality. This means that the vector configurations $\mathcal{U}_{\boldsymbol{k}}$ and $\mathcal{U}_{\bar{\boldsymbol{k}}}$ are *dual as oriented matroids.*

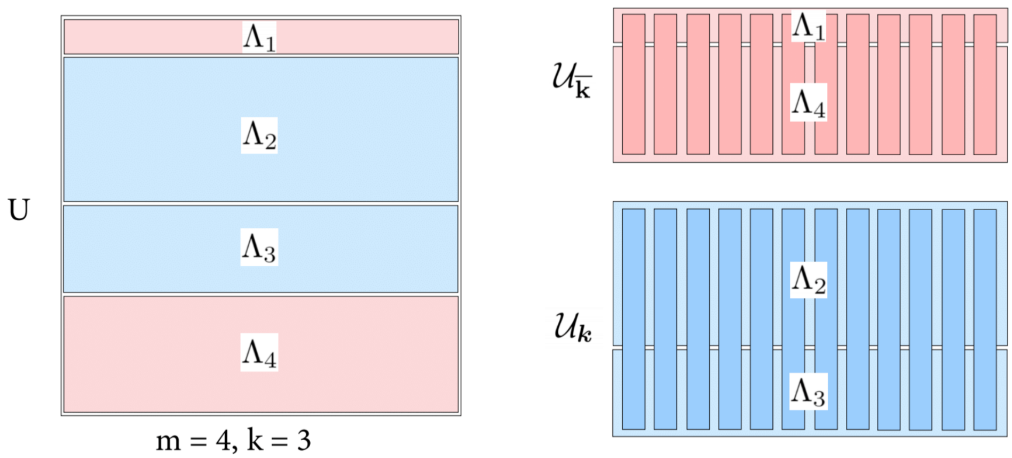


Figure 1.2: A cartoon of the process for arriving at the dual vector configurations $\mathcal{U}_{\boldsymbol{k}}$ and $\mathcal{U}_{\bar{\boldsymbol{k}}}$ from the matrix of eigenvectors U.

Because we further have that the first row of $U_{\bar{\boldsymbol{k}}}$ is $\mathbb{1}$, $P_{\bar{\boldsymbol{k}}} := \operatorname{conv}(\mathcal{U}_{\bar{\boldsymbol{k}}})$ is a polytope lying in the $x_1 = 1$ hyperplane and $0 \in \operatorname{relint}\operatorname{conv}(\mathcal{U}_{\boldsymbol{k}})$. In this situation, the vector configuration $\mathcal{U}_{\boldsymbol{k}}$ is called the *Gale transform* or *Gale diagram* of the polytope $\operatorname{conv}(\mathcal{U}_{\bar{\boldsymbol{k}}})$ ([35], see also [45, 109]). A polytope of the form $P_{\bar{\boldsymbol{k}}}$ is called an *eigenpolytope* of the graph G, a notion first proposed by Godsil [40, 42], and typically used to study the symmetries of a graph through the symmetries of the eigenpolytopes. Gale duality [35] provides the following correspondence between faces of $P_{\bar{\boldsymbol{k}}}$ and linear dependencies of $\mathcal{U}_{\boldsymbol{k}}$.

Theorem 1.2.1. For any $I \subseteq [n]$, there is a positive linear dependence on the vectors in $\mathcal{U}_{\boldsymbol{k}}$ indexed by I if and only if there is a face of $P_{\bar{\boldsymbol{k}}}$ containing all the vectors in $\mathcal{U}_{\bar{\boldsymbol{k}}}$ indexed by $[n] \setminus I$.

1.2.2 Results

Our main structure theorem relating graphical designs to eigenpolytopes is the following consequence of Gale duality. Let $G = ([n], E)$ be a graph with eigenspaces ordered as $\Lambda_1 < \ldots < \Lambda_m$. A vertex subset $S \subseteq [n]$ is a positively weighted k-graphical design if and only if $[n]\backslash S$ indexes all the elements of $\mathcal{U}_{\overline{\boldsymbol{k}}}$ which lie on a face of the eigenpolytope $P_{\overline{\boldsymbol{k}}}$. This follows because positively weighted k-graphical designs are exactly the positive linear dependences on the vectors in $\mathcal{U}_{\boldsymbol{k}}$. This theorem has some variations, namely minimal positively weighted k-graphical designs correspond to facets of the associated eigenpolytope, and arbitrarily weighted k-graphical designs correspond to hyperplanes which may slice through the interior of the associated eigenpolytope.

Since there is a polytope for every choice of k, which must have at least one face, there are positively weighted k-graphical designs for every k. Moreover, we can upper bound the size of a minimum cardinality graphical design, as a polytope must have at least one facet, and the smallest possible facet by number of vertices is a simplex. Specifically, given an eigenspace ordering $\Lambda_1 < \cdots < \Lambda_m$, for every $k = 1, \ldots, m-1$ there is a positively weighted k-design of size at most $\sum_{i=1}^{k} \dim \Lambda_i$. The Gale duality bijection also provides a method to organize graphical designs. Each support minimal design corresponds to a facet, and the non-minimal designs on non-maximal faces correspond to the common coarsening of the designs on all the adjacent facets.

We next apply this result to several families of Cayley graphs. We recall that for a group H and (generating) set $S \subseteq H$ which is closed under taking inverses, the (connected) Cayley graph $\Gamma(H, S)$ has vertex set H, and gh is an edge if $g = sh$ for some $s \in S$. The spectrum of Cayley graphs is well understood through the group characters of H, and this is particularly nice when H is abelian. We first consider the cocktail party graphs $\Gamma(\mathbb{Z}_{2d}, [2d-2])$, which can also be defined as the edge graph of the d-dimensional cross polytope or the complete multipartite graph $K_{2,\ldots,2}$. For any d, this graph has two eigenspaces. We note that the two eigenpolytopes of $\Gamma(\mathbb{Z}_{2d}, [2d-2])$ are the d-simplex and the d-dimensional cross polytope, and use this to fully classify all graphical designs of cocktail party graphs.

We next consider the cycle graphs $\Gamma(\mathbb{Z}_n, \{\pm 1\})$. We show that the extremal eigenpolytope in the frequency ordering depends on the congruence class of $n \mod 4$ and compute the minimal graphical designs in each case, using the fact that the extremal eigenpolytopes are polygons with either 4, $n/2$, or n vertices. I believe these results would extend readily to extremal designs in other orderings.

Lastly we consider the cube $Q_d = \Gamma(\mathbb{Z}_2^d, \{e_i\}_{i=1}^d)$ again. As previously mentioned, for each $v \in \{0,1\}^d$, there is an eigenvector $\varphi_v \in \{\pm 1\}^{\{0,1\}^d}$ whose coordinates are given by $\varphi_v(x) = (-1)^{v^\top x}$ for $x \in \{0,1\}^d$. The eigenspaces of Q_d are naturally indexed by $0, \ldots, d$, where $\Lambda_i = \operatorname{span}\{\varphi_v : \mathbb{1}^\top v = i\}$. We note that this ordering is not the frequency order. The eigenpolytope for Λ_2 is the *cut polytope* $\mathrm{CUT}_d^\square$ [29, 77]. Using results about the *triangular facets* of the cut polytope, we describe all minimum extremal designs with Λ_2 ordered last, which we note are combinatorial. We then consider extremal designs in the frequency order, which essentially orders $\Lambda_{d/2}$ last. Like with the cycle, the exact situation depends on the congruence class of $d \mod 4$. When $d \equiv 2 \mod 4$, we show that the associated extremal eigenpolytope is centrally symmetric, which implies that the minimum extremal designs consist of half the vertices. In the other cases, we provide bounds on the size of a minimum design which are significantly better than the previously mentioned upper bound. We do this by showing that Bonisoli's maximum equidistant linear codes [16] provide small combinatorial designs. We dedicate this result to David Shiroma and Chris Lee, undergraduates at the University of Washington who independently discovered Bonisoli's construction during a research project through the Washington eXperimental Mathematics Lab, which I was a graduate student mentor for.

1.3 Eigenpolytope Universality and Graphical Designs

Chapter 3 is [7], which is joint work with David Shiroma. This paper is under review. We provide a strongly polynomial time algorithm to create a positively weighted graph which has an eigenpolytope that is affinely equivalent to any given polytope. We also extend the

Gale duality bijection between graphical designs and eigenpolytopes to graphs with positive edge weights. Using these two tools, we establish the first complexity results for computing graphical designs.

1.3.1 Background

Positively weighted graphs allow for much greater expressive power than regular, unweighted graphs. However, the Gale duality story of regular graphs does not extend immediately, as the operator AD^{-1} is not symmetric when the graph is irregular. Thus we no longer have a guarantee of orthogonal eigenspaces. We fix this issue by considering graphical designs arising from the eigenspaces of the combinatorial graph Laplacian $D - A$, which is symmetric and positive semidefinite for any positively weighted graph. If the graph is connected, then the eigenspace for $\lambda = 0$ of $D - A$ is spanned by the all-ones vector $\mathbb{1}$. The background on Gale duality developed in Section 1.2.1 then applies directly to the eigenspaces of $D - A$.

1.3.2 Results

We begin by showing that the eigenpolytopes of positively weighted graphs are universal, in the sense that any polytope up to affine equivalence may appear as the eigenpolytope of a positively weighted graph. We do this in two steps. We first show the following.

Lemma 1.3.1. Let $\mathcal{B} = \{\varphi_1 = \mathbb{1}, \varphi_2, \ldots, \varphi_n\}$ be a rational, orthogonal basis of $\mathbb{R}^n$, partitioned as $\mathcal{B} = \pi_1 \sqcup \ldots \sqcup \pi_m$ with at least two parts such that $\pi_1 = \{\mathbb{1}\}$. There is a connected, positively weighted graph $G = ([n], E, w)$, $w \in \mathbb{Q}^E_{>0}$ with m Laplacian eigenspaces $\Lambda_1, \ldots, \Lambda_m$ such that π_i spans Λ_i. The graph G can be constructed in strongly polynomial time.

Our algorithm takes in a basis of $\mathbb{R}^n$ satisfying these properties, and perturbs the unweighted complete graph in a way that preserves the positive edge weights and separates the eigenspaces according to the desired partition. The constructed graph is always dense. The proof reveals a polyhedral structure underlying the eigenvalues which define a positively weighted graph for a given basis. We then use this algorithm to show the following.

Lemma 1.3.2. Let P be a d-dimensional polytope given as the convex hull of n rational vertices. We can create a connected, positively weighted graph $G = ([n], E, w), w \in \mathbb{Q}^E_{<0}$ which has an eigenpolytope that is affinely equivalent to P in strongly polynomial time.

We start with a polytope $P = \text{conv}(\{v_1, \dots, v_n\})$. We first center this polytope at the origin and perform Gram-Schmidt orthogonalization on the rows of the matrix

$$\begin{bmatrix} & \mathbb{1}^\top & \\ v_1 & \dots & v_n \end{bmatrix} \in \mathbb{Q}^{(d+1)\times n}.$$

We can find a rational, orthogonal basis of the null space of this matrix in strongly polynomial time using Gaussian elimination. All together, these vectors are then a rational, orthogonal basis of $\mathbb{R}^n$ which satisfies the hypothesis of Lemma 1.3.1 using a partition into three parts, corresponding to the span of $\mathbb{1}$, the polytope P, and the 'leftovers' from the null space calculation. Hence we can create a positively weighted graph with three eigenspaces, and the eigenpolytope of the eigenspace created from P is affinely equivalent to P by construction.

We next extend the main structure theorem of [6] as follows. Let $G = ([n], E, w)$ be a positively weighted graph with the eigenspaces of $D - A$ ordered as $\Lambda_1 < \ldots < \Lambda_m$. We let U denote the matrix whose rows are the eigenvectors of $D - A$ arranged by eigenspace, and split U into two submatrices: $U_{\boldsymbol{k}}$, which consists of the rows corresponding to $\Lambda_2, \dots, \Lambda_k$, and $U_{[m]\backslash \boldsymbol{k}}$, which consists of all the other rows. We denote the vector configurations arising from the columns of these matrices by $\mathcal{U}_{\boldsymbol{k}}$ and $\mathcal{U}_{[m]\backslash \boldsymbol{k}}$ respectively, and let $P_{[m]\backslash \boldsymbol{k}}$ denote the polytope which is $\text{conv}(\mathcal{U}_{[m]\backslash \boldsymbol{k}})$. A vertex subset $S \subset [n]$ is a positively weighted k-graphical design if and only if $[n]\backslash S$ indexes all the elements of $\mathcal{U}_{[m]\backslash \boldsymbol{k}}$ which lie on a face of the eigenpolytope $P_{[m]\backslash \boldsymbol{k}}$.

The same consequences as in Chapter 2 hold. We have an immediate proof of the existence of positively weighted k-designs for every k and an upper bound on the size of a support minimum positively weighted k-graphical design from the geometry of polytopes. Specifically, given an eigenspace ordering $\Lambda_1 < \ldots < \Lambda_m$ of $D - A$, for every $k = 1, \dots, m-1$ there is a positively weighted k-design of size at most $\sum_{i=1}^k \dim \Lambda_i$. We can also organize the positively weighted k-graphical designs of a positively weighted graph on the facial structure of the eigenpolytope in the same way as with regular graphs. We note that these results subsume the case of regular, unweighted graphs; for a d-regular, unweighted graph, the operators $D - A = dI - A$ and $AD^{-1} = (1/d)A$ differ only by an invertible affine transformation, and hence have the same eigenspaces.

Lemma 1.3.2 shows that every polytope up to affine equivalence with n vertices appears as the eigenpolytope of a positively weighted graph on n vertices. Furthermore, our algorithms show that we can construct a graph with a given eigenpolytope in strongly polynomial time, thus we can translate polytope complexity questions into graphical design complexity questions through Gale duality. We recall that a polytope is simplicial if every facet is a simplex. It was shown in the 1980's that it is NP-complete to determine whether a polytope described by its vertices is simplicial [23, 30, 33], and that it is #P-complete to count the number of facets of a polytope described by its vertices [30, 62]. An immediate consequence of the first result is that it is NP-hard to find the facet of a polytope containing the most vertices of the original polytope, as such an algorithm would detect whether a polytope is simplicial or not. Translating to graphical designs, we have the following three theorems.

Theorem 1.3.3. The following decision problem is strongly NP-complete.

Instance: A connected, positively weighted graph $G = ([n], E, w), w \in \mathbb{Q}^E_{>0}$ with m Laplacian eigenspaces $\Lambda_1 = \text{span}\{\mathbb{1}\} < \ldots < \Lambda_m$, and $k \in \{2, \ldots, m-1\}$.

Question: Is there a positively weighted k-graphical design consisting of fewer than $\sum_{i=1}^k \dim(\Lambda_i)$ vertices?

Theorem 1.3.4. The following problem is NP-hard.

Input: A connected, positively weighted graph $G = ([n], E, w)$, $w \in \mathbb{Q}^E_{>0}$ with m Laplacian eigenspaces $\Lambda_1 = \text{span}\{\mathbb{1}\} < \ldots < \Lambda_m$, and $k \in \{2, \ldots, m-1\}$.

Output: A minimum cardinality positively weighted k-graphical design.

Theorem 1.3.5. The following counting problem is #P-complete.

Input: A connected, positively weighted graph $G = ([n], E, w), w \in \mathbb{Q}^E_{>0}$ with m eigenspaces $\Lambda_1 = \text{span}\{\mathbb{1}\} < \ldots < \Lambda_m$, and an integer $k \in \{2, \ldots, m-1\}$.

Output: The number of minimal positively weighted k-graphical designs of G.

Theorem 1.3.3 follows because this upper bound on the size of a design is tight if and only if every facet of the eigenpolytope is a simplex, which is to say the eigenpolytope is simplicial. We also provide a linear program that finds graphical designs with a guaranteed sparseness.

Chapter 2

GRAPHICAL DESIGNS AND GALE DUALITY

This chapter is the content of [6], written with Rekha Thomas.

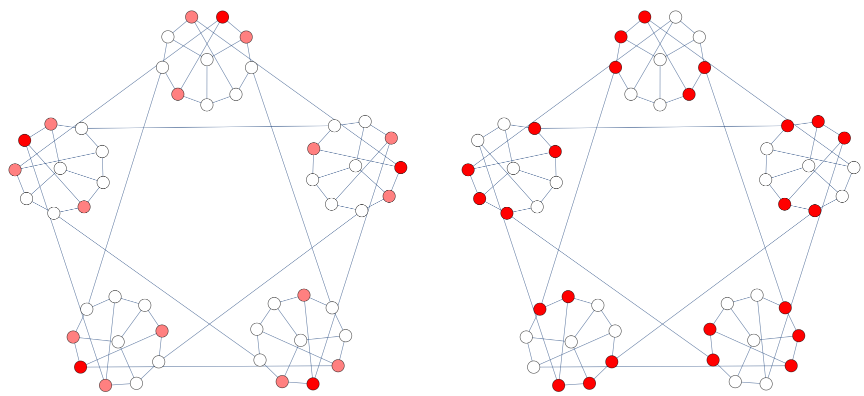
2.1 Introduction

Graphical designs extend classical quadrature rules to the domain of graphs. Informally, a quadrature rule is a set of points on a domain which represent that domain well in terms of numerical integration. That is, the integral of a suitably smooth function over the domain equals a weighted sum of the function values at the quadrature points. A graphical design is a subset of vertices of a graph which approximates the graph in a similar sense; the average of suitable functions over the whole graph agrees with the weighted sum of the function's values on the design.

In this chapter we consider graphical designs in connected regular graphs. A function on a graph $G = (V, E)$ is a map $\varphi : V \to \mathbb{R}$, which we identify with the vector $(\varphi(v) : v \in V) \in \mathbb{R}^V$. The eigenvectors of the normalized adjacency matrix of a graph $G = (V, E)$ form a basis for all function on G. In this chapter, we often use the *frequency order* on eigenspaces which is aligned with a notion of "smoothness" of functions on G. Given any ordering of the eigenspaces, we define a subset of vertices $W \subseteq V$, with weights $(a_w : w \in W)$, to be a *weighted k-design* in G if for all vectors φ in the first k eigenspaces,

$$\sum_{w \in W} a_w \varphi(w) = \frac{1}{|V|} \sum_{v \in V} \varphi(v).$$

By imposing different requirements on the weights a_w, we obtain different types of designs — weighted ($a_w \in \mathbb{R}$), positively weighted ($a_w \geq 0$) or combinatorial ($a_w \in \{0, 1\}$). A design is *extremal* if it averages all eigenspaces except the last one in the given eigenspace ordering.



(a) (b)

Figure 2.1: The Szekeres Snark has 50 vertices, 75 edges and 11 eigenspaces. (A) is a positively weighted 8-design and (B) is a combinatorial 8-design. Lighter reds correspond to smaller weights.

Figure 2.1 depicts positively weighted and combinatorial designs in the 3-regular Szekeres Snark graph that average the first 8 eigenspaces of the normalized adjacency matrix of this graph in frequency order.

In this chapter we show that *Gale duality* [35], from the theory of polytopes, creates a bijection between the positively weighted k-designs in a graph and the faces of a generalized *eigenpolytope* of the graph. Eigenpolytopes were defined by Godsil [40], and we extend their definition for our purposes. This connection, and a more general connection to *oriented matroid duality*, allows one to organize, compute and optimize graphical designs using the combinatorics of the corresponding eigenpolytope. In Figure 2.2, we see an illustration of the design-face correspondence for extremal designs on the octohedral graph with the eigenspace for $\lambda = -1/2$ ordered last.

We use our main result to compute and/or bound the minimal positively weighted extremal designs in three well-known families of Cayley graphs. For cocktail party graphs, which are the edge graphs of cross-polytopes, we show that every minimal weighted ex-

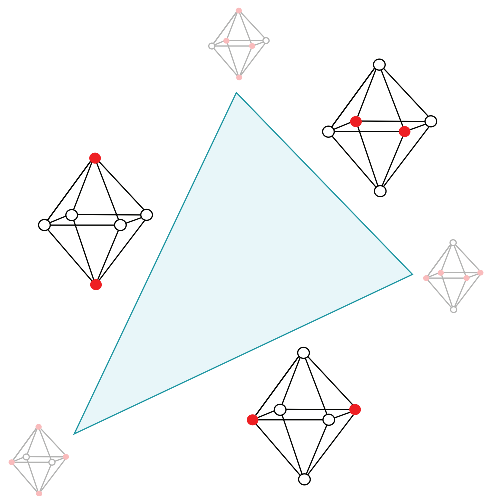


Figure 2.2: The eigenpolytope for $\lambda = -1/2$ of the octahedron is a triangle. The three facets are in bijection with the three minimal positively weighted designs in the octahedron in the eigenspace ordering that puts $\lambda = -1/2$ last. The vertices of the triangle correspond to non-minimal designs given by the union of the two adjacent minimal designs.

tremal design (in any ordering) is combinatorial, and we describe them explicitly. For cycles, we show that every minimal weighted extremal design in the frequency order is positively weighted, and find their sizes. For the edge graph of a d-hypercube and frequency order, we give a precise description of extremal designs for when $d \equiv 2 \bmod 4$. For the other congruence classes, we bound the size of a minimal extremal design. The cube results rely on the theory of linear codes.

Graphical designs were defined relatively recently, by Steinerberger in [96]. He was motivated by spherical designs and more generally, designs in manifolds. The main result of [96] is that if W is a "good" graphical design, then either $|W|$ is large, or the j-neighborhoods of W grow exponentially. In [61], Steinerberger and Linderman give bounds on the numerical integration error for any quadrature rule on a graph. Golubev in [43] introduced extremal designs and connected them to extremal combinatorics. Babecki in [5] refined the definition of graphical designs to make sense when the eigenvalues of a graph Laplacian have multiplicity, connected linear codes in the Boolean cube to graphical designs in the edge graphs of hypercubes, and distinguished graphical designs from a handful of related concepts in the adjacent literature. She also hosts a database of examples and code at `https://sites.math.washington.edu/~GraphicalDesigns/`.

Modern data is often best modeled through graphs, driving an increasingly important need for new data processing tools in graphs. The relatively new field of *graph signal processing* (see, for instance, [75, 76, 79, 3, 102, 100, 12, 24, 48, 67, 88]) seeks to extend classical signal processing techniques to the domain of graphs. Graphical designs offer a framework for *graph sampling*, a notoriously difficult problem in applied mathematics. A concrete connection between graphical designs and graph sampling was established recently in [97, Section 3]. Graphical designs also connect to pure mathematics and theoretical computer science through combinatorics, spectral graph theory, error correcting codes, probability, Fourier analysis, and representation theory.

This chapter is organized as follows. Section 2.2 states the formal definitions of designs and illustrates their nuances through examples. Section 2.3 introduces the necessary background on Gale duality and proves our main structure theorem connecting graphical designs to the facial structure of eigenpolytopes. We then illustrate the subtleties and power of this result through several further examples. Section 2.3 concludes with an overview of the eigenpolytope literature and a rephrasing of the main results of Golubev [43] in terms of eigenpolytopes. In Section 2.4, we use Gale duality to classify the minimal positively weighted extremal designs in two families of graphs, the n-cycle and cocktail party graphs. Section 2.5 considers edge graphs of d-dimensional hypercubes, which we denote by Q_d. We describe the eigenpolytopes of Q_d, one of which is the cut polytope. Facets of the cut polytope given by triangle inequalities can be used to find the minimum extremal designs in a particular eigenspace ordering of Q_d. Under frequency order, we prove upper bounds on the size of a smallest positively weighted extremal design for Q_d using Gale duality and linear codes; these bounds are tight when $d \equiv 2 \mod 4$.

Acknowledgments. We thank Sameer Agarwal and Stefan Steinerberger for many useful discussions and suggestions. We also thank Chris Lee and David Shiroma, undergraduates at the University of Washington, who worked with us in Autumn 2021 on graphical designs. They independently discovered the construction in Bonisoli's theorem on linear codes which provides strong bounds on extremal designs in the graphs of hypercubes. We explain this result in Section 2.5.

2.2 Graphical Designs: Definitions and Examples

Let $G = ([n], E)$ be a connected, simple, undirected graph with vertex set $[n] := \{1, \ldots, n\}$ and edge set E. We will assume throughout that G is regular with the degree of every vertex equal to δ. The *adjacency matrix* $A \in \mathbb{R}^{n\times n}$ of G is defined by $A_{ij} = 1$ if $ij \in E$ and $A_{ij} = 0$ otherwise. Let $D \in \mathbb{R}^{n\times n}$ be the diagonal matrix with $D_{ii} = \deg(i) = \delta$, where $\deg(i)$ is the degree of vertex $i \in [n]$. Then the spectrum of the *normalized adjacency matrix* $AD^{-1} = (1/\delta)A$ is contained in the interval $[-1, 1]$, and 1 is an eigenvalue of AD^{-1}. We denote the eigenspace of 1 by Λ_1. In general, the dimension of Λ_1 is the number of connected components of G, and in our set up, $\Lambda_1 := \operatorname{span}\{\mathbb{1}\}$, where $\mathbb{1}$ denotes the all-ones vector.

Throughout this chapter, we will refer to the spectral information of AD^{-1} as the spectral information of G. We will use the eigenvalues and eigenspaces of AD^{-1} to define graphical designs in G. We note that in [96], graphical designs were defined using the normalized Laplacian matrix $AD^{-1} - I$. Since $AD^{-1} - I$ and AD^{-1} have the same eigenspaces with eigenvalues shifted by 1, we use the simpler AD^{-1} in this chapter. An eigenvector of AD^{-1} will be interpreted as a function $\varphi : V \to \mathbb{R}$, with the v-th coordinate denoted by $\varphi(v)$. We begin by defining what it means for a subset of vertices to *average* an eigenspace Λ of G.

Definition 2.2.1. Let $G = ([n], E)$ be a graph. A subset of vertices $W \subseteq [n]$ *averages the eigenspace* Λ of G if there are weights $(a_w \in \mathbb{R} : w \in W)$ such that for every eigenvector φ in a basis of Λ,

$$\sum_{w\in W} a_w \varphi(w) = \frac{1}{n}\sum_{v\in[n]} \varphi(v). \tag{2.1}$$

There are three types of weights of interest in this chapter: arbitrary ($a_w \in \mathbb{R}$), positive ($a_w > 0$), and uniform ($a_w = 1/|W|$). In classical numerical integration, negative weights are undesirable as they can lead to divergent solutions and numerical instability, see, for instance [51]. The main results of this chapter are about positively weighted graphical designs.

If G is regular, then AD^{-1} is symmetric, so we can find a set of n orthogonal eigenvectors that form a basis for $\mathbb{R}^n$. It will be convenient to not assume that the eigenvectors have unit length, allowing us to use $\mathbb{1}$ as the eigenvector spanning Λ_1. The average of $\mathbb{1}$ over G is

$$\frac{1}{n}\sum_{v\in[n]} 1 = 1. \tag{2.2}$$

If φ is an eigenvector of AD^{-1} with eigenvalue not equal to 1, then $\mathbb{1}^\top\varphi = 0$ by orthogonality. Hence the average of φ over G is

$$\frac{1}{n}\sum_{v\in[n]} \varphi(v) = \frac{1}{n}\mathbb{1}^\top\varphi = 0. \tag{2.3}$$

Therefore, we may interpret the weights in (2.1) as a vector a orthogonal to φ with $a_i = 0$ for all $i \notin W$ and $a_i = a_w$ for all $i = w \in W$. Suppose G has m eigenspaces, and fix an ordering with $\Lambda_1 = \text{span}\{\mathbb{1}\}$ ordered first. A weighted k-graphical design is a subset of vertices that averages the first k eigenspaces in this ordering.

Definition 2.2.2 (k-graphical designs)**.** Suppose $G = ([n], E)$ has m eigenspaces ordered as $\text{span}\{\mathbb{1}\} = \Lambda_1 < \ldots < \Lambda_m$.

1. A *weighted k-graphical design* of G is a subset $W \subseteq [n]$ and weights $(a_w \in \mathbb{R} : w \in W)$ such that W averages the eigenspaces $\Lambda_1, \ldots, \Lambda_k$.

2. If in addition, $a_w > 0$ for all $w \in W$, we call W a *positively weighted k-graphical design* of G, and

3. if $a_w = 1/|W|$, then we call W a *combinatorial k-graphical design* of G.

We often drop the word 'graphical' and refer to k-designs. The different types of weights provide a hierarchy of k-designs: any combinatorial k-design is a positively weighted k-design, and any positively weighted k-design is a weighted k-design. In general, the three types of weights provide distinct designs as we will see shortly. For later use, it will be convenient to characterize the different types of designs as follows. The *support* of a vector $a \in \mathbb{R}^n$ is $\text{supp}(a) := \{i \in [n] : a_i \neq 0\}$. For a subset $W \subset [n]$, define $\mathbb{1}_W$ by $\mathbb{1}_W(i) = 1$ if $i \in W$ and 0 otherwise.

Lemma 2.2.3. Suppose $G = ([n], E)$ has m distinct eigenspaces ordered as

$$\text{span}\{\mathbb{1}\} = \Lambda_1 < \ldots < \Lambda_m.$$

1. $W \subseteq [n]$ is a weighted k-design of G if and only if there is a non-zero vector $a \in \mathbb{R}^n$ such that
$$W = \text{supp}(a), \quad \varphi^\top a = 0 \;\; \forall \varphi \in \Lambda_2, \ldots, \Lambda_k, \quad \mathbb{1}^\top a \neq 0.$$

2. $W \subseteq [n]$ is a positively weighted k-design of G if and only if there is a non-zero vector $a \in \mathbb{R}^n, a \geq 0$ such that
$$W = \text{supp}(a) \text{ and } \varphi^\top a = 0 \;\; \forall \varphi \in \Lambda_2, \ldots, \Lambda_k.$$

3. $W \subseteq [n]$ is a combinatorial k-design of G if and only if $\varphi^\top \mathbb{1}_W = 0 \;\; \forall \varphi \in \Lambda_2, \ldots, \Lambda_k$.

Proof. The proof of this lemma mostly follows from (2.3). The only extra piece is the condition that $\mathbb{1}^\top a \neq 0$ in (1). This is because $W = \text{supp}(a)$ averages $\Lambda_1 = \text{span}\{\mathbb{1}\}$ if and only if $\mathbb{1}^\top a = 1$. If a is a non-zero vector orthogonal to all vectors in $\Lambda_2, \ldots, \Lambda_k$ for which $\mathbb{1}^\top a \neq 0$, then we can scale it to get $\mathbb{1}^\top a = 1$ while preserving the orthogonality requirements. This proves (1). The statements in (2) and (3) do not need this condition to be stated explicitly since if $a \neq 0$ and $a \geq 0$ or $a \in \{0, 1\}^n$ then it follows that $\mathbb{1}^\top a \neq 0$. $\square$

We note a quick fact about combinatorial designs.

Lemma 2.2.4. If $W \subset [n]$ is a combinatorial k-design, then so is $[n] \setminus W$.

Proof. Let $\varphi \in \bigcup_{i=2}^{k} \Lambda_i$. If W is a combinatorial k-design, $\mathbb{1}_W \in \{0,1\}^n$ and $\varphi^\top \mathbb{1}_W = 0$. Since $\varphi \perp \mathbb{1}$, $\varphi^\top \mathbb{1}_{[n]\setminus W} = \varphi^\top(\mathbb{1} - \mathbb{1}_W) = 0$. Hence $[n] \setminus W$ is also a combinatorial k-design. $\square$

A natural quest at this point is to find the smallest graphical designs that can average as many eigenspaces as possible, given a fixed eigenspace ordering. We first note that no proper subset of $[n]$ can average all eigenspaces of G.

Lemma 2.2.5. In a connected, regular graph $G = (V, E)$, no proper subset $W \subset V$ can average all eigenspaces of G in any eigenspace ordering with any type of weights.

Proof. Suppose $W \subset [n]$ averages every eigenspace of G. Let U be a matrix whose rows form a basis for $\Lambda_2 \oplus \cdots \oplus \Lambda_m$. By (2.3), $W = \text{supp}(a)$ for some $a \in \ker U$, which is 1-dimensional and spanned by $\mathbb{1}$. Therefore, $a = \mathbb{1}/n$ and $\text{supp}(W) = V$. $\square$

This brings us to the next two definitions.

Definition 2.2.6 (Maximal and Extremal Designs)**.** Suppose G has m eigenspaces with a fixed ordering $\text{span}\{\mathbb{1}\} = \Lambda_1 < ... < \Lambda_m$, and let $k_{\max}$ be maximal such that G has a $k_{\max}$-graphical design.

1. A *maximal design* in G is a $k_{\max}$-graphical design.

2. An *extremal design* in G is an $(m-1)$-graphical design.

Note that the maximal and extremal designs of a graph depend on the eigenspace ordering chosen. We show in Section 2.3 that every graph has a positively weighted extremal design. However, a graph may have no extremal combinatorial designs.

Example 2.2.7. Let $G = ([12], E)$ be the edge graph of a regular icosahedron. We record a basis for each eigenspace Λ_i of G (with eigenvalue λ_i) in Figure 2.3.

$\lambda_1 = 1$	1	1	1	1	1	1	1	1	1	1	1	1
	ϕ	$-\phi$	$-\phi$	ϕ	-1	-1	1	1	0	0	0	0
$\lambda_2 = -.4472$	-1	1	ϕ	$-\phi$	0	ϕ	$-\phi$	0	0	-1	1	0
	ϕ	$-\phi$	-1	1	0	$-\phi$	ϕ	0	-1	0	0	1
	ψ	$-\psi$	$-\psi$	ψ	-1	-1	1	1	0	0	0	0
$\lambda_3 = .4472$	-1	1	ψ	$-\psi$	0	ψ	$-\psi$	0	0	-1	1	0
	ψ	$-\psi$	-1	1	0	$-\psi$	ψ	0	-1	0	0	1
	-1	-1	1	1	0	0	0	0	0	0	0	0
	-1	-1	0	0	0	1	1	0	0	0	0	0
$\lambda_4 = -.2$	-1	-1	0	0	1	0	0	1	0	0	0	0
	-1	-1	0	0	0	0	0	0	0	1	1	0
	-1	-1	0	0	0	0	0	0	1	0	0	1

Figure 2.3: The rows of this matrix form an eigenbasis of the icosahedral graph. The horizontal lines divide the eigenspaces for the eigenvalues $\lambda_1, \lambda_2, \lambda_3, \lambda_4$. Here $\phi = (1+\sqrt{5})/2$ and $\psi = (1-\sqrt{5})/2$.

Suppose we order the eigenspaces of G as $\Lambda_1 < \Lambda_4 < \Lambda_3 < \Lambda_2$. Then, G has no extremal combinatorial designs; Figure 2.4 shows the minimum cardinality positively weighted 2-designs for this ordering, which are also combinatorial. There are 12 minimum cardinality arbitrarily weighted 3-designs, each consisting of 7 vertices. A minimum cardinality positively weighted 3-design consists of 9 vertices, see Figures 2.5A,B. These computations were done in Matlab [68].

However, in the ordering $\Lambda_1 < \Lambda_2 < \Lambda_3 \leq \Lambda_4$, a minimum cardinality 3-design is combinatorial and consists of only 2 vertices. Every 2-vertex 3-design in this ordering consists of a pair of antipodal points on the icosahedron (see Figure 2.5C). $\square$

Example 2.2.7 brings up the question of eigenspace ordering. Different orderings on

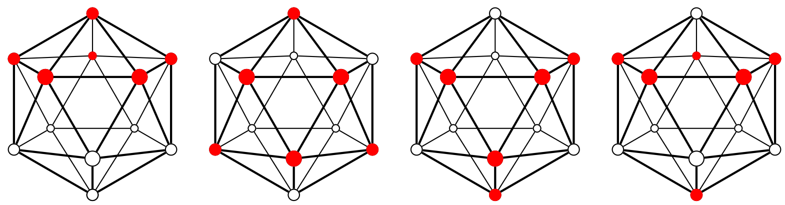
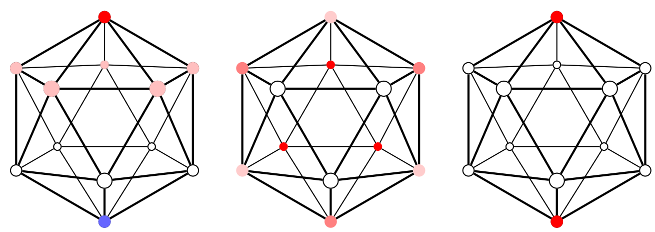


Figure 2.4: The isomorphism classes of the minimum cardinality positively weighted 2-design with eigenspace ordering $\Lambda_1 < \Lambda_4 < \Lambda_3 < \Lambda_2$. These are also combinatorial designs.



(a) (b) (c)

Figure 2.5: Three extremal designs of the icosahedral graph. Figures A and B show the isomorphism classes of the minimum weighted and positively weighted designs respectively for $\Lambda_1 < \Lambda_4 < \Lambda_3 < \Lambda_2$. Figure C shows the isomorphism class of the minimum weighted design for $\Lambda_1 < \Lambda_2 < \Lambda_3 \leq \Lambda_4$, which is combinatorial. Lighter colors correspond to weights of smaller magnitude, red indicates positive and blue is negative.

the eigenspaces of G produce different graphical designs. A physically motivated ordering on eigenspaces is the *frequency ordering*, first introduced in [96]. The distinct eigenvalues $\lambda_1, \ldots, \lambda_m$ of G are ordered by decreasing absolute value; i.e.,

$$1 = |\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_n| \geq 0.$$

This induces an ordering on the eigenspaces $\Lambda_1, \ldots, \Lambda_m$ of G, though there may be ties. In particular, the spectrum of every bipartite graph is symmetric about 0, which leads to some ambiguity. We denote $\Lambda_i < \Lambda_j$ when $|\lambda_i| > |\lambda_j|$, and $\Lambda_i \leq \Lambda_j$ when we have chosen to break a tie by ordering Λ_i before Λ_j. In Figure 2.3, the eigenspaces are labeled by frequency.

The frequency ordering comes from an analogy to spherical harmonics. The matrix AD^{-1} is a Laplacian-type operator, which for regular graphs is in many senses analogous to the spherical Laplacian on $\mathbb{S}^{n-1}$ (see [49, 20, 92], for instance). The frequency ordering on the eigenspaces of AD^{-1} captures a similar notion of smoothness and symmetry that low degree spherical harmonics capture for the sphere. In this sense, graphical designs with the frequency ordering on eigenspaces extend spherical quadrature rules to the discrete domain of graphs.

2.3 Oriented Matroids and Eigenpolytopes

In this section we establish our main structure theorem which shows that there is a bijection between positively weighted k-designs in a graph and the faces of a generalized *eigenpolytope* of the graph. This result bestows a great deal of combinatorial structure on k-designs, allowing polyhedral methods to find, organize, and optimize them. The theorem is derived via *Gale duality* from the theory of polytopes which lives under the bigger umbrella of oriented matroid duality of vector configurations. We begin with some background.

2.3.1 Oriented matroid duality of vector configurations

We introduce vector configurations and their oriented matroid duality tailored to our needs, along the lines of [109, Chapter 6]. Suppose $\mathcal{U} = \{u_1, \ldots, u_n\} \subset \mathbb{R}^{n-(d+1)}$ is a collection of vectors such that the matrix $U = \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix} \in \mathbb{R}^{(n-(d+1))\times n}$ has rank $n-(d+1)$. The *dual configuration* to $\mathcal{U}$ is the collection $\mathcal{U}^* = \{u_1^*, \ldots, u_n^*\} \subset \mathbb{R}^{d+1}$ such that the rows of the matrix

$$U^* = \begin{bmatrix} u_1^* & u_2^* & \cdots & u_n^* \end{bmatrix} \in \mathbb{R}^{(d+1)\times n}$$

form a basis for the nullspace of U. Equivalently, $U(U^*)^\top = 0$ and $\operatorname{rank}(U^*) = d+1$. Assume further that $\mathbb{1}$ is the first row of U^*. Then the following hold: (i) the convex hull of $\mathcal{U}^*$, denoted as $\operatorname{conv}(\mathcal{U}^*)$, is a polytope of dimension d in $\mathbb{R}^{d+1}$ lying in the hyperplane $x_1 = 1$, and (ii) $\mathcal{U}$ satisfies the *positive dependence* relation $\sum u_i = 0$. A *dependence* on a set of vectors is a linear combination of the vectors that equals 0, and the dependence is *positive* if all coefficients in the combination are non-negative.

Definition 2.3.1. 1. A vector $c \in \mathbb{R}^n$ is a *circuit* of the configuration $\mathcal{U}$ (or the matrix U) if $c \neq 0$, $Uc = 0$ and $\operatorname{supp}(c)$ is inclusion minimal with these properties. A circuit c of $\mathcal{U}$ is *positive* if $c \geq 0$.

2. The *cocircuits* of $\mathcal{U}$ (or the matrix U) are the non-zero vectors $v^\top U$ of minimal support. A cocircuit $v^\top U$ of $\mathcal{U}$ is *positive* if $v^\top U \geq 0$.

The circuits of $\mathcal{U}$ are the minimal non-zero dependences of $\mathcal{U}$, or equivalently, the minimally sparse non-zero vectors in the nullspace of U. Similarly, the cocircuits of $\mathcal{U}$ are the minimally sparse non-zero vectors in the row space of U. Since the nullspace of U is the row space of U^*, the circuits of $\mathcal{U}$ are precisely the cocircuits of $\mathcal{U}^*$ and vice-versa. In this sense the configurations $\mathcal{U}$ and $\mathcal{U}^*$ are dual.

We refer to [45, 109] for the basics of polyhedral theory. Here are the basic definitions that we will need. A *polytope* P in $\mathbb{R}^\ell$ is the convex hull of a finite set of points in $\mathbb{R}^\ell$, and its dimension is the dimension of the affine span of these points. A (proper) *face* of a full-dimensional polytope $P \subset \mathbb{R}^\ell$ is the intersection $P \cap \mathcal{H} \neq \emptyset$, where $\mathcal{H} \subset \mathbb{R}^\ell$ is a hyperplane that contains P in one of its closed halfspaces. A *facet* of P is a face of P of dimension $\dim(P) - 1$, and a *vertex* of P is a face of dimension 0. The proper faces of P along with P and the empty set are all the faces of P, and all faces of a polytope are again polytopes. An ℓ-dimensional polytope has at least $\ell + 1$ vertices.

There is a remarkable bijection between the positive dependences of $\mathcal{U}$ and the faces of the polytope $\operatorname{conv}(\mathcal{U}^*)$ as stated below, see [45, p. 88].

Theorem 2.3.2 (Gale Duality)**.** For any $I \subseteq [n]$, $\operatorname{conv}\{u_i^* : i \in [n] \setminus I\}$ is a face of $\operatorname{conv}(\mathcal{U}^*)$ if and only if 0 is in the relative interior of $\operatorname{conv}\{u_i : i \in I\}$.

For $I \subseteq [n]$, 0 is in the relative interior of $\operatorname{conv}\{u_i : i \in I\}$ if and only if there is a $c \geq 0$ such that $\operatorname{supp}(c) = I$ and $Uc = 0$, which is if and only if c is a positive dependence of $\mathcal{U}$ with $\operatorname{supp}(c) = I$. This yields the following corollary.

Corollary 2.3.3. For any $I \subseteq [n]$, $\operatorname{conv}\{u_i^* : i \in [n] \setminus I\}$ is a face (facet) of $\operatorname{conv}(\mathcal{U}^*)$ if and only if I is the support of a positive dependence (circuit) of $\mathcal{U}$.

It is customary to use the index set $J \subseteq [n]$ to denote both the collection $\{u_j : j \in J\}$ and the polytope $\operatorname{conv}\{u_j : i \in J\}$.

Example 2.3.4. A classic illustration of Theorem 2.3.2 is given by the dual configurations $\mathcal{U}$ and $\mathcal{U}^*$ shown in Figure 2.6, derived from

$$U = \begin{bmatrix} 1 & 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad U^* = \left[\begin{array}{cccccc} 1 & 1 & 1 & 1 & 1 & 1 \\ \hline 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{array}\right]$$

for which $n = 6$ and $d = 3$. Here $\operatorname{conv}(\mathcal{U}^*)$ is an octahedron lying on the plane $x_1 = 1$ in

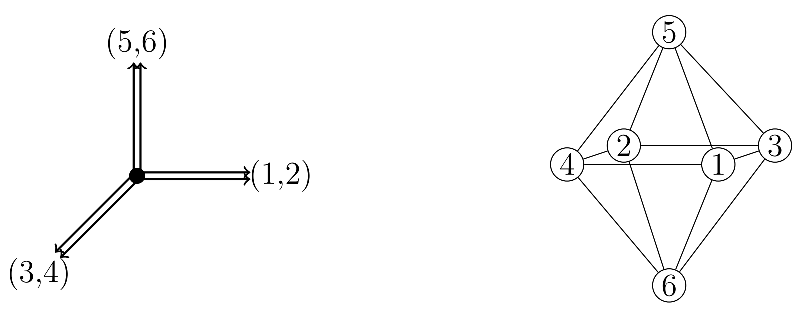


Figure 2.6: The configuration $\mathcal{U}$ and the octahedron $\operatorname{conv}(\mathcal{U}^*)$.

$\mathbb{R}^4$. The configuration $\mathcal{U} \subset \mathbb{R}^2$ has 6 positive circuits. The complements of their supports index the six facets of the octahedron. For example, $\{1, 3, 5\}$ is a positive circuit of $\mathcal{U}$ and its complement $\{2,4,6\}$ is a facet of $\mathrm{conv}(\mathcal{U}^*)$. The vector $(0,0,0,0,1,-1)$ is a circuit of $\mathcal{U}$ but since it is not positive, its complement $\{1,2,3,4\}$ is not a face of the octahedron; it is a cocircuit of $\mathcal{U}^*$ and corresponds to a hyperplane slicing through the interior of the octahedron. □

2.3.2 Graphical designs and oriented matroid duality

We now connect graphical designs to oriented matroid and Gale duality. Assume that the m eigenspaces of G have been ordered as $\Lambda_1 < \cdots < \Lambda_m$, with $\Lambda_1 = \mathrm{Span}\{\mathbb{1}\}$, $d_i := \dim(\Lambda_i)$ and $s_k := \sum_{i=1}^k d_i$. Let $U \in \mathbb{R}^{n\times n}$ be a matrix whose rows are a set of n orthogonal eigenvectors of G. For any collection of eigenvalues $\boldsymbol{\lambda} = \{\lambda_{i_1}, \ldots \lambda_{i_j}\}$ of G, let $U_{\boldsymbol{\lambda}}$ denote the submatrix of U whose rows (in order) are the eigenbases of Λ_i for $i \in \boldsymbol{\lambda}$.

Suppose we are interested in the k-designs of G in this ordering for some $k < m$. Let $\mathbf{k} = \{\lambda_2, \ldots, \lambda_k\}$ and $\overline{\mathbf{k}} = \{\lambda_1, \lambda_{k+1}, \ldots, \lambda_m\}$. Then $U_{\boldsymbol{k}}$ and $U_{\overline{\mathbf{k}}}$ partition U into two submatrices, each with n columns, and $\mathbb{1}$ is the first row of $U_{\overline{\mathbf{k}}}$. The configuration $\mathcal{U}_{\boldsymbol{k}} \subset \mathbb{R}^{s_k-1}$ is dual to the configuration $\mathcal{U}_{\overline{\mathbf{k}}} \subset \mathbb{R}^{n-s_k+1}$ in the sense of Section 2.3.1. Keep in mind that $\mathcal{U}_{\boldsymbol{k}}$ and $\mathcal{U}_{\overline{\mathbf{k}}}$ are ordered vector configurations and not sets, and hence allow for repeated elements.

Lemma 2.3.5. The following hold.

1. $P_{\overline{\mathbf{k}}} := \mathrm{conv}(\mathcal{U}_{\overline{\mathbf{k}}})$ is a $(n-s_k)$-dimensional polytope in $\mathbb{R}^{(n-s_k)+1}$ lying on the hyperplane $x_1 = 1$.

2. The circuits of $\mathcal{U}_{\mathbf{k}}$ are in bijection with the cocircuits of $\mathcal{U}_{\overline{\mathbf{k}}}$.

3. The positive circuits of $\mathcal{U}_{\mathbf{k}}$ are in bijection with the facets of $P_{\overline{\mathbf{k}}}$.

The polytope $P_{\overline{\mathbf{k}}}$ is a generalized version of an *eigenpolytope* of a graph, defined by Godsil in [40].

Definition 2.3.6. [40] Let λ be an eigenvalue of G, U_λ be a matrix whose rows form a basis of the eigenspace Λ_λ, and $\mathcal{U}_\lambda$ be the collection of columns of U_λ. Then the polytope $P_\lambda := \text{conv}(\mathcal{U}_\lambda)$ is the *eigenpolytope* of G with respect to λ.

Even though the definition of an eigenpolytope is dependent on the choice of a basis of the eigenspace, eigenpolytopes are well defined up to combinatorial type, which is all that matters here. Indeed, the eigenpolytopes defined from two different bases of an eigenspace differ by an invertible linear transformation which preserves combinatorial structure. There is a rich literature on eigenpolytopes which we will comment on at the end of this section.

The polytopes of interest to us are of the form $P_{\overline{\mathbf{k}}}$ (as in Lemma 2.3.5) that correspond to multiple eigenvalues of G including $\lambda_1 = 1$. To address them, we generalize Definition 2.3.6 as follows.

Definition 2.3.7. Let $\boldsymbol{\lambda} = \{\lambda_{i_1}, \ldots, \lambda_{i_l}\}$ be a set of eigenvalues of G and $U_{\boldsymbol{\lambda}}$ be the submatrix of U consisting of the eigenvectors associated to $\boldsymbol{\lambda}$. Define $\mathcal{U}_{\boldsymbol{\lambda}}$ to be the vector configuration of the n columns of $U_{\boldsymbol{\lambda}}$ and $P_{\boldsymbol{\lambda}} := \text{conv}(\mathcal{U}_{\boldsymbol{\lambda}})$. The polytope $P_{\boldsymbol{\lambda}}$ is an *eigenpolytope* of G associated to $\boldsymbol{\lambda}$.

We now have all the tools to state our main structure theorem.

Theorem 2.3.8. Let $G = ([n], E)$ be a graph with eigenspaces ordered as $\Lambda_1 < \ldots < \Lambda_m$, let $W \subseteq [n]$ be a subset of the vertices of G, and let $k < m$. Consider the dual configurations $\mathcal{U}_{\boldsymbol{k}}$ and $\mathcal{U}_{\overline{\boldsymbol{k}}}$ as defined before. Then W is a (minimal) positively weighted k-design of G if and only if the convex hull of the subset of $\mathcal{U}_{\overline{\boldsymbol{k}}}$ indexed by $[n]\backslash W$ is a (facet) face of $P_{\overline{\boldsymbol{k}}} = \text{conv}(\mathcal{U}_{\overline{\boldsymbol{k}}})$.

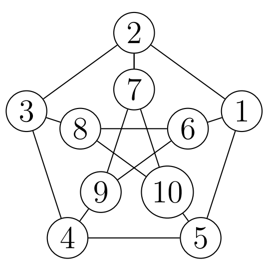
Proof. By Lemma 2.2.3 (2), W is a (minimal) positively weighted k-design of G if and only if $W = \text{supp}(a)$ for a positive (circuit) dependence a of $\mathcal{U}_{\boldsymbol{k}}$. The statement now follows from Corollary 2.3.3. $\square$

Remark 2.3.9. The positively weighted k-designs of minimum cardinality correspond to the facets of $P_{\overline{\boldsymbol{k}}}$ that contain the maximum number of columns of $U_{\overline{\boldsymbol{k}}}$. If all columns of $U_{\overline{\boldsymbol{k}}}$

are vertices of $P_{\overline{\boldsymbol{k}}}$, then the positively weighted k-designs of minimum cardinality correspond to the facets of $P_{\overline{\boldsymbol{k}}}$ with the maximum number of vertices.

Though it could be difficult to find the facet of a polytope containing the most vertices, we will see that this strategy is successful in examples.

Example 2.3.10. The **Petersen graph** shown in Figure 2.7 has three eigenvalues $\lambda_1 = 1^{(1)}, \lambda_2 = (-2/3)^{(4)}$, and $\lambda_3 = (1/3)^{(5)}$, listed in frequency order, with multiplicity recorded as exponents. The eigenpolytopes of the Petersen graph for individual eigenvalues were studied in [77] and [82].



$$U_{\overline{\mathbf{2}}} = \left[\begin{array}{cccccccccc} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ \hline 0 & -1 & 0 & 1 & 1 & 0 & -1 & 0 & 0 & 0 \\ 1 & -1 & -1 & 0 & 1 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 1 & -1 & 0 \\ 0 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & -1 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \end{array}\right]$$

Figure 2.7: The Petersen graph.

Suppose we want to know the minimal positively weighted extremal designs of G in frequency order. By Theorem 2.3.8, we compute $\overline{\mathbf{2}} = \{1, 3\}$ and the matrix $U_{\overline{\mathbf{2}}}$ whose first row is a basis for Λ_1 and next 5 rows form a basis for Λ_3. The eigenpolytope $P_{\overline{\mathbf{2}}}$ is the convex hull of $\mathcal{U}_{\overline{\mathbf{2}}}$. This is a 5-dimensional polytope with 10 vertices, 22 facets and face-vector $(10, 45, 90, 75, 22)$. The 22 facets come in two symmetry classes. There are 10 facets with 6 vertices and 12 facets that are 4-simplices. Therefore, there are 10 minimal positively weighted extremal designs with $4 = 10 - 6$ elements and 12 minimal positively weighted extremal designs with $5 = 10 - 5$ elements. The two types of designs are shown in Figure 2.8. $\square$

(a) (b)

Figure 2.8: The minimal positively weighted extremal designs on the Petersen graph with $\Lambda_1 < \Lambda_2 < \Lambda_3$ (up to isomorphism). Figure A gives the design from a simplicial facet of $P_{\{1,3\}}$ and is combinatorial. Figure B gives the design from a 6-vertex facet and needs positive weights of two different types.

Theorem 2.3.8 provides a natural adjacency structure on the minimal positively weighted k-designs of G: two such designs are adjacent if the facets of $P_{\overline{\mathbf{k}}}$ that index them meet on a ridge (a face of codimension 2). Therefore, the adjacency graph of minimal positively weighted k-designs is precisely the edge skeleton of the polytope polar to $P_{\overline{\mathbf{k}}}$. This observation is subsumed by the general fact that the faces of $P_{\overline{\mathbf{k}}}$ (and hence also the faces of the polar polytope) index the positively weighted k-designs of G. Thus one can assign (non-minimal) positively weighted k-designs to the edges of the adjacency graph which we can think of as a common coarsening of the minimal designs on the two vertices of the edge. More precisely, if there are two adjacent minimal positively weighted k-designs $W = \operatorname{supp}(a)$ and $W' = \operatorname{supp}(a')$, then so is $W \cup W'$ since $U_{\boldsymbol{k}}(a + a') = 0$ and $a + a' \geq 0$. The non-minimal design $W \cup W'$ lives on the edge joining W and W'.

Example 2.3.11. We zoom in on the adjacency graph of the minimal positively weighted extremal designs of the Petersen graph. Figure 2.9 shows the neighborhood of the minimal design $W = \{1, 2, 3, 4, 5\}$. On the edges one sees non-minimal designs as explained above.

Next we show an example in which the eigenpolytope $P_{\boldsymbol{\lambda}}$ can be much simpler than what

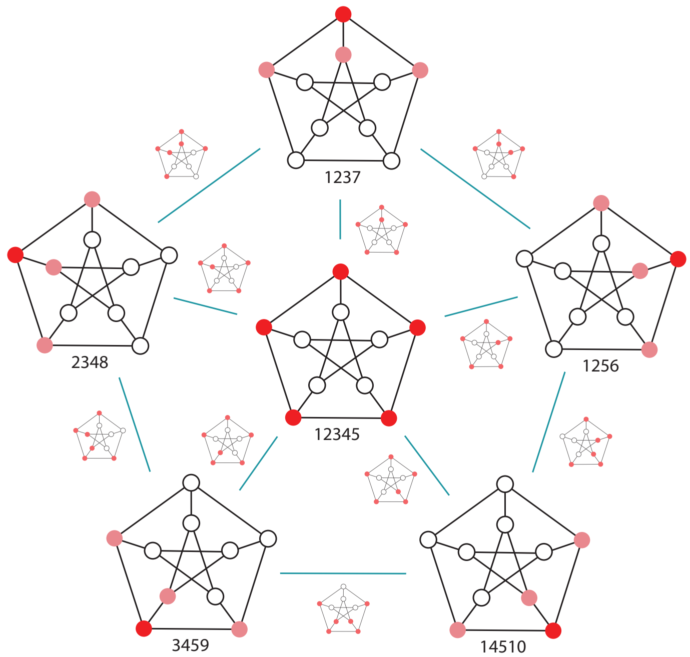


Figure 2.9: The minimal extremal positively weighted designs of the Petersen graph adjacent to $\{1, 2, 3, 4, 5\}$, and the non-minimal positively weighted extremal designs connecting them.

the size of $U_{\boldsymbol{\lambda}}$ predicts. This happens when $U_{\boldsymbol{\lambda}}$ has repeated columns which can dramatically cut down the number of vertices of $P_{\boldsymbol{\lambda}}$.

Example 2.3.12. Let $G = ([12], E)$ be the **truncated tetrahedral graph** (see Figure 2.10). The eigenvalues of G in frequency order are

$$\lambda_1 = 1^{(1)}, \lambda_2 = 2/3^{(3)}, \lambda_3 = -2/3^{(3)}, \lambda_4 = -1/3^{(3)}, \lambda_5 = 0^{(2)}.$$

We look again at minimal positively weighted extremal designs in this graph which are all 4-designs. Recall that $\mathbf{4} = \{\lambda_2, \lambda_3, \lambda_4\}$ and $\overline{\mathbf{4}} = \{\lambda_1, \lambda_5\}$. We compute

$$U_{\bar{\mathbf{4}}} = \left[\begin{array}{cccccccccccc} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ \hline 1 & -1 & 0 & 0 & -1 & 1 & 1 & -1 & 0 & -1 & 1 & 0 \\ 0 & -1 & 1 & 1 & -1 & 0 & 0 & -1 & 1 & -1 & 0 & 1 \end{array}\right].$$

Since each column of $U_{\bar{\mathbf{4}}}$ is repeated four times, $P_{\bar{\mathbf{4}}} \simeq \Delta_2$ is a triangle, shown in Figure 2.10, with each vertex labeled by the indices of the four columns of $U_{\bar{\mathbf{4}}}$ that coincide with that vertex.

Consider the facet (edge) of $P_{\bar{\mathbf{4}}}$ defined by the vertices with labels $\{3, 4, 9, 12\}$ and $\{1, 6, 7, 11\}$. The complimentary index set is $\{2, 5, 8, 10\}$. By Theorem 2.3.8, $W = \{2, 5, 8, 10\}$ is a minimal positively weighted 4-design on the truncated tetrahedral graph. Moreover, there are exactly 3 such designs, one for each facet of $P_{\bar{\mathbf{4}}}$.

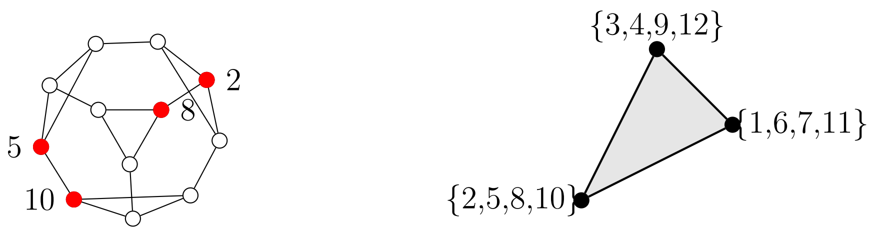


Figure 2.10: A minimal positively weighted 4-design and the eigenpolytope $P_{\bar{\mathbf{4}}}$ of the truncated tetrahedral graph.

In this example,

$$U_{\mathbf{4}} = \left[\begin{array}{cccccccccccc}
-1 & -1.5 & -0.5 & 1.5 & 2 & 1.5 & -0.5 & -1.5 & -1 & 1 & 0 & 0 \\
2 & 1.5 & 1.5 & -0.5 & -1 & -1.5 & -1.5 & -0.5 & -1 & 0 & 1 & 0 \\
-1 & -0.5 & -1.5 & -1.5 & -1 & -0.5 & 1.5 & 1.5 & 2 & 0 & 0 & 1 \\
\hline
0 & -1 & 1 & -1 & 0 & 1 & -1 & 1 & 0 & 0 & 0 & 0 \\
-1 & 0 & 1 & -1 & 1 & 0 & 0 & 0 & 0 & -1 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & -1 & 1 & 0 & -1 & -1 & 0 & 1 \\
\hline
-1 & 0 & 1 & 0 & -1 & 0 & 1 & 0 & -1 & 1 & 0 & 0 \\
-1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & 1 & 0 \\
-1 & 1 & 0 & 0 & -1 & 1 & 0 & 0 & -1 & 0 & 0 & 1
\end{array}\right].$$

The circuit associated with the design $W = \{2, 5, 8, 10\}$ is $e_2 + e_5 + e_8 + e_{10}$, a 0/1 vector, i.e., $U_{\mathbf{4}}\mathbb{1}_W = 0$. Therefore, W is also combinatorial. $\square$

Gale duality has traditionally been used to understand the facial structure of a polytope by analyzing the vector configuration dual to the vertices of the polytope. The dual configuration is called the *Gale dual* of the polytope. This has been especially successful when the Gale dual configuration lies in a low-dimensional space, and many surprising properties of polytopes have been discovered through Gale duality (see [109, Chapter 6], [45]). In this chapter we propose using Gale duality in the reverse direction, namely, use the combinatorics of eigenpolytopes to understand positively weighted graphical designs. This is especially effective when the eigenpolytope is easy to understand. We already saw this in action in Example 2.3.12 where the eigenpolytope was just a triangle. Here is a bigger example to drive home this strategy of using polytopes to inform designs.

Example 2.3.13. Let $G = ([48], E)$ be the **truncated cuboctahedral graph** shown in Figure 2.11. This graph has 17 eigenvalues, listed below in frequency order, with exponents showing their multiplicities:

$$1^{(1)}, -1^{(1)}, 0.9107^{(3)}, -0.9107^{(3)}, 0.7810^{(3)}, -0.7810^{(3)}, 2/3^{(2)}, -2/3^{(2)}, 0.6045^{(3)},$$
$$-0.6045^{(3)}, 1/3^{(4)}, -1/3^{(4)}, 0.2440^{(3)}, -0.2440^{(3)}, 0.1569^{(3)}, -0.1569^{(3)}, 0^{(4)}$$

The matrix $U_{\overline{\mathbf{16}}}$ is made up of 8 horizontally concatenated copies of

$$\left[\begin{array}{cccccc} 1 & 1 & 1 & 1 & 1 & 1 \\ \hline 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 & 0 \end{array}\right].$$

For an index set $I \subseteq [6]$, let $C(I) = \{j \in [48] : j \equiv i \mod 6 \text{ for some } i \in I\}$, that is, all vertices of G indexing the columns of $U_{\overline{\mathbf{16}}}$ that correspond to columns indexed by I of the above matrix. For example, $C(\{1\}) = \{1, 7, 13, 19, 25, 31, 37, 43\}$.

Using Polymake [38], we find that the four-dimensional polytope $P_{\overline{\mathbf{16}}}$, which has only 6 vertices, has 8 facets indexed by the following collections of vertices:

$$C(\{3,4,5,6\}), C(\{2,4,5,6\}), C(\{2,3,4,5\}), C(\{1,2,3,5\}),$$
$$C(\{1,2,3,4\}), C(\{1,3,5,6\})C(\{1,2,4,6\}), C(\{1,2,5,6\}).$$

By Theorem 2.3.8, G has eight minimal positively weighted extremal designs which we can read off from the complements of the vertex labels of a facet. For instance, the facet $C(\{3,4,5,6\})$ is a certificate that

$$C(\{1,2\}) = \{1,2,7,8,13,14,19,20,25,26,31,32,37,38,43,44\}$$

indexes a minimal positively weighted extremal design, which also happens to be a combinatorial design. We exhibit this graphical design in Figure 2.11.

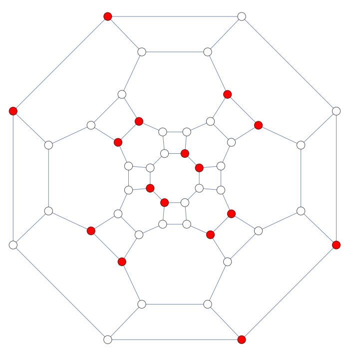


Figure 2.11: A minimal extremal combinatorial design on the truncated cuboctohedral graph.

The facets of the polytope $P_{\overline{\mathbf{16}}}$ are easy to list and analyze, whereas a brute force enumeration of the circuits of $U_{\mathbf{16}}$ is computationally taxing. Beginning at $t = 8$, it exceeds MATLAB's [68] preset size restrictions to check whether each t-element subset of [48] is a circuit. Even if we knew to look only at 16-element subsets, there are roughly $2.255 \cdot 10^{12}$ of them. $\square$

Gale duality provides a simple upper bound on the size of positively weighted designs. This answers an eigenspace version of open question #6 posed in [96].

Theorem 2.3.14. Let G be a graph with eigenspaces ordered as $\Lambda_1 < \Lambda_2 < \cdots < \Lambda_m$, $\dim \Lambda_i = d_i$, and $s_k := \sum_{i=1}^{k} d_i$. Then for every $k = 1, \ldots, m-1$ there is a positively weighted k-design of size at most s_k. In particular, there is a positively weighted extremal design of size at most $s_{m-1} = n - d_m$.

Proof. The eigenpolytope $P_{\bar{\mathbf{k}}}$ has dimension $\sum_{i=k+1}^{m} d_i = n - s_k$. Therefore any facet has at least $n - s_k$ distinct vertices and at most $n-1$ vertices. By Theorem 2.3.8, the size of any minimal positively weighted k-design lies between s_k and 1. □

Remark 2.3.15. The bijection between k-designs of G and the faces of the eigenpolytope $P_{\bar{\mathbf{k}}}$ of G provides a cursory upper bound on the maximum number of minimal positively weighted designs through the upper bound theorem for convex polytopes [70]. Specifically, if $P_{\bar{\mathbf{k}}}$ is d-dimensional, then there are at most

$$\binom{n - \lfloor \frac{d+1}{2} \rfloor}{n-d} + \binom{n - \lfloor \frac{d+2}{2} \rfloor}{n-d}$$

minimal positively weighted k-graphical designs of G.

In practice, there is often a preference for positive weights in quadrature rules. By *Caratheodory's theorem* [21], generically, the smallest (arbitrarily) weighted k-designs have size s_k. Theorem 2.3.14 shows that for each k, there are *positively* weighted k-designs of size at most s_k, illustrating that positive weights are not too restrictive. The short proof is an immediate consequence of the Gale connection. There are graphs where the upper bound in Theorem 2.3.14 is tight for every k.

Example 2.3.16. Consider again the icosahedral graph from Example 2.2.7 with $\Lambda_1 < \Lambda_4 < \Lambda_3 < \Lambda_2$. In this ordering, $s_1 = 1, s_2 = 6, s_3 = 9$. Any single vertex is a 1-design (in any graph). We saw that a minimum cardinality positively weighted 2-design is combinatorial and has $s_2 = 6$ vertices, and a minimum cardinality positively weighted 3-design has $s_3 = 9$ vertices.

Theorem 2.3.14 does not provide a general lower bound, as a facet may have $n-1$ vertices. There are indeed single vertex k-graphical designs when $k > 1$.

Example 2.3.17. Consider the second Loupekines Snark, pictured in Figure 2.12, and label the distinguished red vertex as 1. The eigenspace Λ_2 of this graph is 2-dimensional and is contained in $e_1^\perp$. Therefore, for $W = \{1\}$ and $\varphi \in \Lambda_2$, we have $e_1^\top \varphi = 0$ which means that $W = \{1\}$ averages Λ_2. $\square$

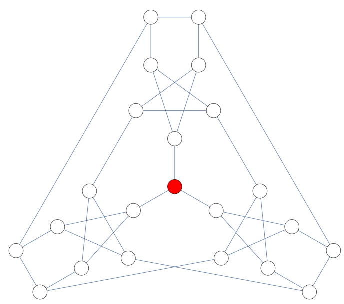


Figure 2.12: A combinatorial 2-graphical design on the second Loupekines Snark.

We close this subsection by commenting on weighted designs that are not positively weighted. Lemma 2.2.3 (1) says that W is a weighted k-design of G if and only if $W = \operatorname{supp}(a)$ for some dependence a of $U_{\boldsymbol{k}}$ with $\mathbb{1}^\top a \neq 0$. Recall that if $U_{\boldsymbol{k}} a = 0$, then a lies in the row space of $U_{\overline{\boldsymbol{k}}}$ and hence, $a = v_a^\top U_{\overline{\boldsymbol{k}}}$ for some v_a. We can think of a as the vector of values of the linear functional $v_a^\top y$ on the elements of $\mathcal{U}_{\overline{\boldsymbol{k}}}$ (keeping repetitions) which contain among them the vertices of $P_{\overline{\boldsymbol{k}}}$. Let $\mathcal{H}_{v_a}$ be the hyperplane

$$\mathcal{H}_{v_a} := \{y \in \mathbb{R}^{n-s_k+1} \, : \, v_a^\top y = 0\}.$$

The weighted k-design given by a is $W = \operatorname{supp}(a)$, and $i \in W$ if and only if the ith element of $\mathcal{U}_{\overline{\boldsymbol{k}}}$ does not lie on $\mathcal{H}_{v_a}$. If $a \geq 0$ then all of $\mathcal{U}_{\overline{\boldsymbol{k}}}$ lies in one halfspace of $\mathcal{H}_{v_a}$ and therefore also, the eigenpolytope $P_{\overline{\boldsymbol{k}}}$. If a is a non-positive dependence, then there are elements of $\mathcal{U}_{\overline{\boldsymbol{k}}}$ in both open halfspaces of $\mathcal{H}_{v_a}$ and the hyperplane $\mathcal{H}_{v_a}$ intersects the interior of $P_{\overline{\boldsymbol{k}}}$. When a is a circuit of $\mathcal{U}_{\boldsymbol{k}}$, the hyperplane $\mathcal{H}_{v_a}$ is a visualization of the corresponding cocircuit of $\mathcal{U}_{\overline{\boldsymbol{k}}}$. We illustrate on two graphs.

Example 2.3.18. Consider again the icosahedral graph from Example 2.2.7 with $\Lambda_1 < \Lambda_4 < \Lambda_3 < \Lambda_2$. By [42, Theorem 4.3], the eigenpolytope P_{λ_2} is the icosahedron again. Hyperplanes defined by circuits corresponding to minimum cardinality weighted and positively weighted 3-designs with respect to $\Lambda_1 < \Lambda_4 < \Lambda_3 < \Lambda_2$ are shown in Figure 2.13. The first hyperplane intersects P_{λ_2} in its interior.

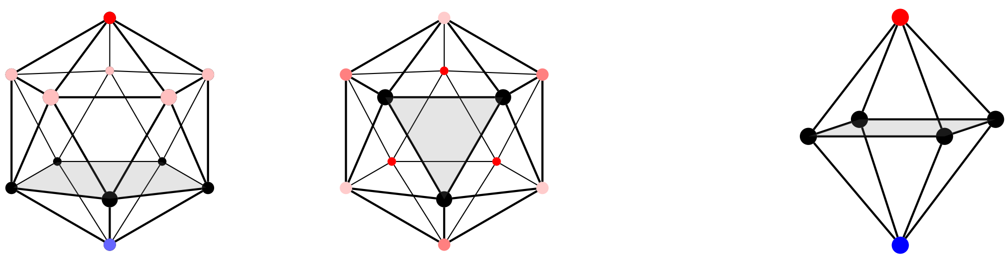


Figure 2.13: Hyperplanes corresponding to circuits.

One has to be careful when dealing with non-positively weighted designs since in that case, a dependence a gives rise to a graphical design if and only if $\mathbb{1}^\top a \neq 0$. Consider the graph of the regular octahedron in Figure 2.13. By [42, Theorem 4.3] again, the eigenspace of $\lambda = 0$ is an octahedron. From Example 2.3.4, $a = (0, 0, 0, 0, 1, -1)$ is a circuit and the corresponding hyperplane bisects the octahedron as shown. However $\mathbb{1}^\top a = 0$, and so this circuit a fails to average Λ_1.

$\square$

2.3.3 Eigenpolytope Literature

Eigenpolytopes of a graph G with respect to single eigenvalues were defined by Godsil in [40]. He used the symmetries of eigenpolytopes to understand $\mathrm{Aut}(G)$, the automorphism group of G. Our eigenpolytopes in Definition 2.3.7 are more general in that they involve sets of eigenvalues, and using them to study graphical designs is new.

Most of the existing work on eigenpolytopes focuses on the second largest eigenvalue of the adjacency matrix A, which they term θ_1. The eigenpolytope P_{θ_1} is often closely tied to the structure and symmetry of G; most notably for distance regular graphs [42, 83]. We also refer the reader to further work on symmetry and families of graphs in [22, 85, 82]. Padrol and Pfeifle [77] translate graph operations to operations on eigenpolytopes arising from the graph Laplacian $D - A$. They mention in passing that eigenpolytopes might connect to oriented matroids and Gale duality. For regular graphs, the eigenspaces of A, AD^{-1}, $D - A$, and many other common graph matrices are equivalent.

The n columns of the matrix U_λ whose rows form a basis for the eigenspace of λ can be thought of as an embedding of the n vertices of G. In some situations the edge graph of the eigenpolytope $P_\lambda = \operatorname{conv}(\mathcal{U}_\lambda)$ is isomorphic to G and provides a *spectral drawing* of G, see [107, 108, 41, 84] for more on this connection. McConnell in [69] computes an extensive list of spectral graph drawings of the graphs of uniform polyhedra. Eigenpolytopes corresponding to multiple eigenvalues are, in spirit, analogous to spectral drawings using eigenvectors of multiple eigenvalues.

2.3.4 Connections to Extremal Combinatorics

The extremal designs found by Golubev in [43] provide classes of faces of certain eigenpolytopes. We rephrase his results in our language. We first recall the *Hoffman bound*, which does not actually appear in the standard reference [50]. The origins and generalizations of this theorem are explained in [47]. If G is strongly regular, the linear programming bound of [27] is the Hoffman bound.

Theorem 2.3.19. (Hoffman Bound [47]) Let G be a regular graph on n vertices, let $\lambda_{\min}$ be the least eigenvalue of AD^{-1}, and let $\alpha(G)$ be the size of a maximum stable set of G. Then,

$$\frac{\alpha(G)}{n} \leq \frac{-\lambda_{\min}}{1 - \lambda_{\min}}.$$

The following theorem is a translation of [43, Theorem 2.2] to eigenpolytopes.

Theorem 2.3.20. Let G be a regular graph for which the Hoffman bound is sharp. Then, a maximum stable set and its complement each provide a face of $P_{\lambda_{\min}}$.

Proof. Let $G = (V, E)$ have the eigenspace of $\lambda_{\min}$ ordered last. By [43, Theorem 2.2] and [5, Theorem 5.6], a maximum stable set $W \subseteq V$ is an extremal combinatorial design, and $V \setminus W$ is an extremal combinatorial design as well by Lemma 2.2.4. By Gale duality, it follows that W and $V \setminus W$ index faces of $P_{\lambda_{\min}}$. □

A *cut* in a connected graph $G = (V, E)$ is a partition of the vertex set V into a set $W \subset V$ and its complement. An edge $ij \in E$ is a *cut edge* in the cut induced by W if one endpoint is in W and the other in $V \setminus W$. We use $E(W, V \setminus W)$ to denote the set of cut edges in the cut induced by W. The second main result of [43] relies on the following variant of the Cheeger bound.

Theorem 2.3.21. ([2, 101]) *Let G be a connected δ-regular graph and θ_1 be the second largest eigenvalue of AD^{-1}. Then*

$$\min_{\varnothing \neq W \subsetneq V} \frac{|V||E(W, V \setminus W)|}{\delta |W||V \setminus W|} \geq 1 - \theta_1.$$

Theorem 2.3.22. Let G be a graph for which the Cheeger bound is sharp. Then, a set which realizes the Cheeger bound and its complement each provide a face of P_{θ_1}.

Proof. Let $G = (V, E)$ have the eigenspace of θ_1 ordered last. By [43, Theorem 2.4] and [5, Theorem 5.11], a set $W \subset V$ realizing the Cheeger bound is an extremal combinatorial design, and hence so is $V \setminus W$ by Lemma 2.2.4. By Gale duality, it follows that W and $V \setminus W$ index faces of P_{θ_1}. □

2.4 *Cocktail Party Graphs and Cycles*

We now use the power of Gale duality via Theorem 2.3.8 to investigate three families of graphs. Since they are all Cayley graphs, we begin with general results about their spectrum which is closely tied to the representation theory of finite groups ([90],[87, Chapter 1]).

Given a group H and a generating set $S \subseteq H$ such that $s \in S \implies s^{-1} \in S$, one can construct the connected, $|S|$-regular Cayley graph $\Gamma(H, S)$. The vertices are indexed by H, and there is an edge between group elements g and h if $g = sh$ for some $s \in S$. The eigenvectors of $\Gamma(H, S)$ are given by the group characters of H. When H is a finite abelian group, this provides a simple method to compute the spectrum of $\Gamma(H, S)$ since there are $|H|$ one-dimensional representations of H. The eigenvalue of an eigenvector φ (a group character of H) can be computed from:

$$(AD^{-1}\varphi)(g) = \frac{1}{|S|}\sum_{h \sim g} \varphi(hg) = \left(\frac{1}{|S|}\sum_{h\sim g}\varphi(h)\right)\varphi(g).$$

The eigenvectors depend only on the group H, but the eigenvalues, and hence groupings of eigenvectors into eigenspaces, depends on the generating set S as well.

2.4.1 The Cocktail Party Graph

We denote the regular *cross-polytope* in dimension d by $\Diamond_d = \operatorname{conv}\{\pm e_i : i \in [d]\}$. Its edge graph is commonly known as the *cocktail party graph* and is a regular graph with $2d$ vertices and degree $2(d-1)$. This graph can also be defined as the *complete multipartite graph* $K_{2,\ldots,2}$, the Cayley graph $\Gamma(\mathbb{Z}_{2d}, [2d-2])$, and the complement of d disjoint copies of the path P_2 with two vertices. In frequency order, the spectrum of the cocktail party graph is

$$1^{(1)}, \left(\frac{-1}{d-1}\right)^{(d-1)}, 0^{(d)};$$

see [19] for a reference. It is quick to compute the matrix U; we label columns by the vertices of $\Diamond_d$, and the row blocks by eigenvalues:

	vertex						
	e_1	$-e_1$	$\cdots$	$\cdots$	$\cdots$	e_d	$-e_d$
$\lambda_1 = 1$				$\mathbb{1}^\top$			
$\lambda_2 = -(d-1)^{-1}$	e_1	e_1	$\cdots$	e_{d-1}	e_{d-1}	$-\mathbb{1}$	$-\mathbb{1}$
$\lambda_3 = 0$	e_1	$-e_1$	$\cdots$	$\cdots$	$\cdots$	e_d	$-e_d$

Theorem 2.4.1. In frequency order, the graph of $\lozenge_d$ has 2^d minimal positively weighted extremal designs, each of which consists of d vertices and corresponds to a facet of $\lozenge_d$. Each of these designs is combinatorial.

Proof. By [42, Theorem 4.3], the eigenpolytope for $\lambda = 0$ is again the cross-polytope $\lozenge_d$, and hence the extremal eigenpolytope $P_{\bar{\mathbf{2}}}$ is isomorphic to $\lozenge_d$. The cross-polytope is simplicial, which is to say that every facet is a d-simplex Δ_{d-1}, which has exactly d vertices. Moreover, a subset of d vertices is a facet of $\lozenge_d$ if and only if its complement is also a facet. Hence, by Theorem 2.3.8, the minimal positively weighted extremal designs of the cocktail party graph consist of $2d - d = d$ vertices, and correspond to the 2^d facets of $\lozenge_d$. Examining the eigenspace Λ_2, it is quick to see that the weight vector for each such design is a 0-1 vector, hence these are combinatorial designs. □

Theorem 2.4.2. With Λ_2 ordered last, the graph of $\lozenge_d$ has d minimal positively weighted extremal designs, each of which consists of 2 antipodal vertices of $\lozenge_d$ and is combinatorial.

Proof. The eigenpolytope P_{λ_2} is Δ_{d-1} with the antipodal vertices of $\lozenge_d$ collapsed into a single vertex of Δ_{d-1}. The complements of facets of Δ_{d-1} are exactly the vertices of Δ_{d-1}. By Theorem 2.3.8, there are d minimal positively weighted extremal designs of $\lozenge_d$ in this ordering of eigenspaces, each of which is a pair of antipodal vertices. Examining the eigenspace Λ_3, it is clear that the weight vector for each such design is of the form $e_i + e_{i+1} \in \mathbb{R}^{2d}$, hence these are combinatorial designs. □

Allowing arbitrary weights, the minimal extremal designs of the cocktail party graph are combinatorial, and in particular, positively weighted.

Theorem 2.4.3. Every minimal weighted extremal design of the cocktail party graph is combinatorial.

Proof. In frequency order, it follows from the structure of the eigenbasis of Λ_2 that if we allow arbitrary weights, then any circuit of U_2 (up to sign) is of the form $a \in \mathbb{R}^{V(\lozenge_d)}$ with

$a_{e_j} = 1$, $a_{-e_j} = -1$ for some j and 0 in all other coordinates. Therefore $\mathbb{1}^\top a = 0$, and $\mathrm{supp}(a)$ is not a graphical design by Lemma 2.2.3 (1). This generalizes the observation in Example 2.3.18. For the other ordering, the hyperplanes $\mathcal{H}$ representing cocircuits of $\mathcal{U}_2$ are precisely the spans of the facets of the eigenpolytope $P_{\lambda_2} = \Delta_d$ which gives combinatorial designs as in Theorem 2.4.2. $\square$

2.4.2 Cycles

We next consider the cycle graph $C_n = \Gamma(\mathbb{Z}_n, \{\pm 1\})$. Let

$$\varphi_j := \begin{bmatrix} 1 \\ \cos(2\pi j/n) \\ \cos(2\pi 2j/n) \\ \vdots \\ \cos(2\pi(n-1)j/n) \end{bmatrix}, \psi_j := \begin{bmatrix} 0 \\ \sin(2\pi j/n) \\ \sin(2\pi 2j/n) \\ \vdots \\ \sin(2\pi(n-1)j/n) \end{bmatrix}.$$

For each $j \in [\lfloor (n-1)/2 \rfloor]$, φ_j and ψ_j span a two-dimensional eigenspace Λ_j of C_n with eigenvalue $\lambda_j = \cos(2\pi j/n)$. If n is even, then $\varphi_{n/2}$ and $\psi_{n/2}$ collapse into the one-dimensional eigenspace $\Lambda_{n/2} = \mathrm{span}\{((-1)^t) : t \in [n]\}$. Therefore, all eigenpolytopes of C_n corresponding to a single eigenvalue (other than $\lambda_1 = 1$) are either a polygon or a line segment. We note that the above indexing of the eigenspaces is not compatible with frequency ordering. In frequency order, the highest frequency eigenspace(s) will correspond to $j \approx n/4$, since $\cos(2\pi j/n) \approx \cos(\pi/2) = 0$. We consider minimal extremal designs of C_n in frequency order and will see that their structure depends on the congruence class of $n \mod 4$.

Theorem 2.4.4. Let $n \equiv 0 \mod 4$. In frequency ordering, C_n has four minimal positively weighted extremal designs, each consisting of $n/2$ vertices. They are
$\{i, i+1 \in [n] : i \equiv j \mod 4\}$ for $j \in [4]$.

Proof. If $n \equiv 0 \mod 4$, then the extremal eigenspace $\Lambda_{n/4}$ with eigenvalue 0 is spanned by

$$\varphi_{n/4} = \begin{bmatrix} 1 \\ \cos(\pi/2) \\ \cos(\pi) \\ \vdots \\ \cos(\pi(n-1)/2) \end{bmatrix} \quad \text{and} \quad \psi_{n/4} = \begin{bmatrix} 0 \\ \sin(\pi/2) \\ \sin(\pi) \\ \vdots \\ \sin(\pi(n-1)/2) \end{bmatrix}.$$

Each element of $\mathcal{U}_{n/4}$ is one of the following:

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ -1 \end{bmatrix}.$$

Thus $P_{n/4}$ is the diamond $\lozenge_2$ with $n/4$ graph vertices indexing each polytope vertex. Each facet is indexed by the vertices $\{i, i+1 \in [n] : i \equiv j \mod 4\}$, and each facet is also the complement of a facet, Thus there are 4 minimal positively weighted extremal designs of the stated form. □

Corollary 2.4.5. Every minimal extremal design of C_n, for $n \equiv 0 \mod 4$, is positively weighted.

Proof. The extremal eigenpolytope of C_n is $\lozenge_2$. By Theorem 2.4.3, the only cocircuit hyperplanes $\mathcal{H}$ that yield designs are the those that support facets of $\lozenge_2$. □

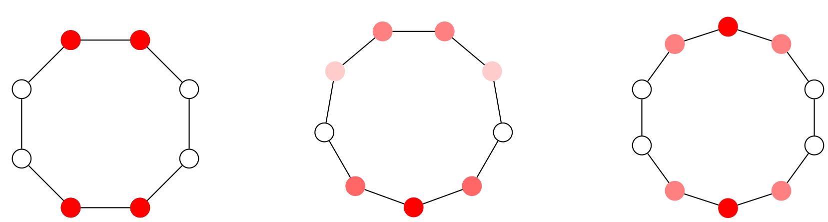


Figure 2.14: Minimal positively weighted extremal designs of C_8, C_9, C_{10}.

For the remaining types of cycles, we need some short gcd calculations.

Lemma 2.4.6. We have the following calculations.

1. If $n \equiv 1 \mod 4$, then $\gcd(n, (n-1)/4) = 1$, $\gcd(2n, (n-1)/2) = 2$, and $\gcd(2n, (n+1)/2) = 1$.

2. If $n \equiv 3 \mod 4$, then $\gcd(n, (n+1)/4) = 1$, $\gcd(2n, (n+1)/2) = 2$, and $\gcd(2n, (n-1)/2) = 1$.

Proof. 1. Let $n = 4k+1$. Then, $k = (n-1)/4$, so

$$\gcd(n, (n-1)/4) = \gcd(k, 4k+1) = \gcd(k, 1) = 1.$$

Since $(n+1)/2 = 2k+1$ is odd,

$$\gcd(2n, (n+1)/2) = \gcd(8k+2, 2k+1) = \gcd(2k+1, 2k-1) = \gcd(2, 2k-1) = 1.$$

Similarly, $(n-1)/2 = 2k$ is even, so

$$\gcd(2n, (n-1)/2) = \gcd(8k+2, 2k) = \gcd(2, 2k) = 2.$$

2. This follows similarly by writing $n = 4k-1$.

□

Theorem 2.4.7. If n is odd, then every minimal positively weighted extremal design of C_n consists of $n-2$ vertices.

Proof. If $n \equiv 1 \mod 4$, the extremal eigenspace $\Lambda_{(n-1)/4}$ with eigenvalue $\cos(\pi(n-1)/4n)$ is spanned by

$$\varphi_{(n-1)/4}(v) = \cos(2\pi v(n-1)/4n) \quad \text{and} \quad \psi_{(n-1)/4}(v) = \sin(2\pi v(n-1)/4n).$$

By Lemma 2.4.6, $\gcd(n, (n-1)/4) = 1$. Thus the values $\cos(2\pi v(n-1)/4n)$ are distinct and $\|(\cos(2\pi v(n-1)/4n), \sin(2\pi v(n-1)/4n))\|_2 = 1$ as v ranges over $[n]$. Therefore, $P_{(n-1)/4}$ is an n-gon, and every facet contains exactly two vertices. The statement about graphical designs then follows from Theorem 2.3.8. The case of $n \equiv 3 \mod 4$ with extremal eigenspace $\Lambda_{(n+1)/4}$ follows similarly. □

Theorem 2.4.8. If $n \equiv 2 \mod 4$, then every minimal extremal design of C_n consists of $n-4$ or $n-2$ vertices depending on which of the eigenspaces indexed by $(n\pm 2)/4$ is ordered last.

Proof. Let $n \equiv 2 \mod 4$. There is a tie for the final eigenspace of C_n in the frequency order, so we consider both $(n \pm 2)/4$. We claim that the extremal eigenpolytope P_m for $m = (n \pm 2)/4$ is the n-gon if m is odd, and is the $(n/2)$-gon doubled up if m is even. Let $n = 2j$, where j is odd. Then $m = (j \pm 1)/2$, and Λ_m is spanned by

$$\varphi_m(v) = \cos(2\pi vm/n) = \cos\left(2\pi v\frac{j\pm 1}{2}/2j\right) \text{ and}$$
$$\psi_m(v) = \sin(2\pi vm/n) = \sin\left(2\pi v\frac{j\pm 1}{2}/2j\right).$$

Suppose m is odd. Then by Lemma 2.4.6, $\gcd(m, n) = 1$, and so the columns of U_m are distinct as v ranges over $[n]$. If m is even, then $\gcd(m, n) = 2$ by Lemma 2.4.6. So, every column of U_m occurs with multiplicity 2, and regardless of the parity of m, every column lies on the unit circle. This proves the claim about P_m.

The doubled $(n/2)$-gon has $n/2$ facets each containing 4 vertices, and the n-gon has n facets each containing 2 vertices. By Theorem 2.3.8, every minimal positively weighted extremal design of C_n then consist of $n-4$ or $n-2$ vertices depending on which of the eigenspaces indexed by $(n \pm 2)/4$ is ordered last. $\square$

Theorem 2.4.9. The minimum cardinality of an arbitrarily weighted extremal design in C_n is achieved by positively weighted extremal designs.

Proof. As noted in several proofs, the vertices of an extremal eigenpolytope P_m lie on the unit circle, and so at most two distinct vertices can lie on a line. This is the same number of distinct vertices on each facet of P_m. $\square$

2.5 *Graphs of Hypercubes*

As our final example, we consider extremal designs in the edge graphs of cubes. Let $Q_d = \Gamma(\{0,1\}^d, \{e_1, \dots e_d\})$ denote the edge graph of the d-dimensional hypercube $[0,1]^d$, which is

d-regular. The Hamming weight of a vector $x \in \{0,1\}^d$ is $|x| := \mathbb{1}^\top x$, the number of 1's in the coordinates of x. For $i = 0, \ldots, d$, let

$$\mathcal{J}_{d,i} = \{x \in \{0,1\}^d \,:\, |x| = i\}$$

be the collection of $\binom{d}{i}$ vertices of Q_d with Hamming weight i. We refer to $\mathcal{J}_{d,i}$ as the i-th slice of the (Boolean) d-cube. It is convenient to index the spectrum of Q_d by the slices of the cube, which differs from frequency ordering.

- The eigenvalues of Q_d are $\lambda_i = 1 - 2i/d$ for $i = 0, \ldots, d$.

- The eigenvalue λ_i has multiplicity $\binom{d}{i} = |\mathcal{J}_{d,i}|$.

- An eigenbasis of the eigenspace of $\lambda_i = 1 - 2i/d$ is given by the vectors

$$\left\{\varphi_x(y) = ((-1)^{x^\top y} \,:\, y \in \{0,1\}^d)^\top \,:\, x \in \mathcal{J}_{d,i}\right\}.$$

The last eigenvalue/eigenspace in frequency order corresponds to the middle level of the cube, $i \approx d/2$. Let P_i denote the eigenpolytope of λ_i.

2.5.1 Eigenpolytopes of the hypercube

For a fixed $i \in \{0, 1, \ldots, d\}$, the matrix U_i has rows indexed by the $\binom{d}{i}$ vectors $x \in \mathcal{J}_{d,i}$, columns by each $y \in \{0,1\}^d$, with (x,y)-entry equal to $(-1)^{x^\top y}$. Let the column indexed by y be denoted as $c(y)$. The eigenpolytope P_i is a full-dimensional polytope in $\mathbb{R}^{\binom{d}{i}}$, and every element of $\mathcal{U}_i$ is a vertex of P_i since they are all ± 1 vectors.

The matrices U_0 and U_d have one row each. Since $U_0 = [\mathbb{1}]$, $P_0 = (\Delta_0)^{2^d}$ is a 0-simplex, i.e., a point, labeled by all elements of $\{0,1\}^d$. The exponent denotes the multiplicity of labels on a vertex of the polytope. The unique row of U_d has entries $c(y) = (-1)^{\mathbb{1}^\top y}$ which records the parity of $|y|$. Therefore $P_d = (\Delta_1)^{2^{d-1}}$ is a line segment with half the elements of $\{0,1\}^d$ labeling each endpoint. Leaving out these eigenpolytopes, we can describe the others.

Lemma 2.5.1. Fix $i \in \{1, \ldots, d-1\}$.

1. If i is odd, then the columns of U_i come in pairs of oppositely signed vectors; $c(y) = -c(\mathbb{1} - y)$ for all $y \in \{0,1\}^d$. The eigenpolytope P_i is a centrally symmetric polytope of dimension $\binom{d}{i}$ with 2^d vertices.

2. If i is even, then the columns of U_i come in pairs of equal vectors; $c(y) = c(\mathbb{1} - y)$ for all $y \in \{0,1\}^d$. The eigenpolytope P_i has dimension $\binom{d}{i}$ and 2^{d-1} vertices. Each vertex has two labels given by the two columns of U_i that give that vertex.

Proof. All of the columns of U_i are vertices of P_i since they are all ± 1 vectors. However, it could be that two or more columns correspond to the same vertex of P_i. Consider the pair of vectors $y \in \{0,1\}^d$ and $\mathbb{1} - y \in \{0,1\}^d$. For $x \in \mathcal{J}_{d,i}$, if $x^\top y = \alpha$, then $x^\top(\mathbb{1} - y) = |x| - \alpha$. Therefore, if $i = |x|$ is odd then α and $|x| - \alpha$ have opposite parity and if $i = |x|$ is even then α and $|x| - \alpha$ have the same parity. So if i is even, $c(y) = c(\mathbb{1} - y)$ and y and $\mathbb{1} - y$ index the same vertex of P_i. If i is odd, $c(y) = -c(\mathbb{1} - y)$, and P_i is centrally symmetric.

To finish the proof, we need to argue that there are no further identifications of columns in U_i. Consider the matrix

$$A = \begin{bmatrix} x_1 & \cdots & x_{\binom{d}{i}} \end{bmatrix}^\top$$

whose rows are made up of the vectors $x_j \in \mathcal{J}_{d,i}$, and partition $\{0,1\}^d$ as $\mathcal{Y} \sqcup \mathcal{Y}'$ so that $y \in \mathcal{Y}$, $\mathbb{1} - y \in \mathcal{Y}'$ and for any $y \in \mathcal{Y}$, $|y| \leq d/2$. By the above, $c(\mathcal{Y}) = \pm c(\mathcal{Y}')$ depending on the parity of i. So, it suffices to show that the map $\varphi : \mathcal{Y} \to \{0,1\}^{\binom{d}{i}}$ given by $\varphi(y) = Ay \bmod 2$ is injective. That is, we want to show there are no linear dependences of A coming from $\mathcal{Y}$. Suppose $Ay = 0$ and $|y| \leq d/2$. Let $I = \operatorname{supp}(y)$. If $|I| \geq 1$, we can find x_j so that $|\operatorname{supp}(x_j) \cap I|$ is odd, since every vector with weight i appears as a row of A. Therefore $x_j^\top y = 1$, a contradiction, and φ is injective. $\square$

Example 2.5.2. Consider Q_3 the edge graph of the 3-cube. The matrix

$$U = \left[\begin{array}{rrrrrrrr} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ \hline 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 \\ \hline 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ \hline 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \end{array}\right]$$

with successive blocks indexed by the eigenvalues ordered by Hamming weight:

$$(\lambda_0 = 1)^1, \left(\lambda_1 = \frac{1}{3}\right)^3, \left(\lambda_2 = -\frac{1}{3}\right)^3, (\lambda_3 = -1)^1.$$

Here are the non-trivial eigenpolytopes of Q_3:

- $i = 1$: P_1 is a centrally symmetric 3-polytope with 8 vertices. It is in fact, a regular 3-cube by [42, Theorem 4.3], which has 6 facets with 4 vertices each. Therefore the smallest positively weighted designs that average all eigenspaces, except the one indexed by λ_1, have size 4.

- $i = 2$: $P_2 = \operatorname{conv}\{(1, 1, 1), (-1, -1, 1), (-1, 1, -1), (1, -1, -1)\} = (\Delta_3)^2$ is a tetrahedron. Each vertex has two labels. Counting this multiplicity of labels, the maximum number of vertices on a facet of P_2 is 6 which implies that the smallest positively weighted designs that average all eigenspaces, except the one indexed by λ_2, have size 2.

2.5.2 The Cut Polytope

Consider the cut in a graph $G = ([d], E)$ induced by a subset S of vertices (c.f. Subsection 2.3.4.) The *incidence vector* of the cut is $\chi_S \in \{0, 1\}^E$ such that $(\chi_S)_{ij} = 1$ if

$ij \in E(S, [d] \setminus S)$, and 0 otherwise. Let K_d be the complete graph on d vertices. The *cut polytope* of K_d, denoted $\mathrm{CUT}_d^\square$, is the convex hull of all incidence vectors of cuts in K_d. The following is possibly well-known and appears in [77] without proof.

Lemma 2.5.3. For the graph Q_d, the eigenpolytope P_2 is isomorphic to $\mathrm{CUT}_d^\square$, the cut polytope of the complete graph K_d on d vertices.

Proof. The (x, y)-entry of U_2 is $c(y)_x = (-1)^{x^\top y} = (-1)^{|\,\mathrm{supp}(x)\,\cap\,\mathrm{supp}(y)|}$, for $x \in \mathcal{J}_{d,2}$, and $y \in \{0,1\}^d$. The vectors x are precisely the incidence vectors of all edges in K_d, and the vectors $y \in \{0,1\}^d$ are the incidence vectors of all possible subsets of $[d]$. Every subset of $[d]$ induces a cut in K_d. We now show that $c(y)_{ij} = -1$ if ij is in the cut induced by $\mathrm{supp}(y)$, and $c(y)_x = 1$ otherwise.

Let $y \in \{0,1\}^d$. If x is an edge of K_d in the cut induced by $\mathrm{supp}(y)$, then $|\,\mathrm{supp}(x) \cap \mathrm{supp}(y)| = 1$, and so $(-1)^{x^\top y} = -1$. If x is not a cut edge, then either $|\,\mathrm{supp}(x) \cap \mathrm{supp}(y)| = 2$ if x indexes an edge contained in $\mathrm{supp}(y)$, or $|\,\mathrm{supp}(x) \cap \mathrm{supp}(y)| = 0$ if x indexes an edge contained in the complement. Either way, $(-1)^{x^\top y} = 1$. Thus $\mathcal{U}_2$ consists of ± 1 vectors indexing cuts in K_d.

We have defined $\mathrm{CUT}_d^\square$ as the convex hull of 0/1 vectors indexing the cuts of K_d. Note that P_2 is the image of $\mathrm{CUT}_d^\square$ under the map $x \mapsto -2x + \mathbb{1}$. $\square$

Since $\chi_S = \chi_{[d]\setminus S}$, the columns of U_2 come in pairs of identical vectors and $P_2 \simeq \mathrm{CUT}_d^\square$ has 2^{d-1} vertices, each corresponding to 2 vectors in $\mathcal{U}_2$. Although the facet structure of $\mathrm{CUT}_d^\square$ is notoriously difficult to understand, its facets with the maximum number of vertices are well understood.

Proposition 2.5.4 (Prop 26.3.12 of [29])**.** For any facet F of $\mathrm{CUT}_d^\square$,

$$|\{\chi_S \in F\}| \leq 3 \cdot 2^{d-3},$$

with equality if and only if F is defined by a triangle inequality.

The *triangle inequalities* are among the simplest facet inequalities of $\mathrm{CUT}_d^\square$, each of the form

$$x_{ij} - x_{ik} - x_{jk} \leq 0 \quad \text{or} \quad x_{ij} + x_{ik} + x_{jk} \leq 2$$

for distinct $i, j, k \in [d]$. By Theorem 2.3.8 and Proposition 2.5.4, the facets of $\mathrm{CUT}_d^\square$ from triangle inequalities are in bijection with the minimum cardinality extremal designs of the graph Q_d with the eigenspace Λ_2 ordered last.

Theorem 2.5.5. Suppose we order the eigenspaces of Q_d, for $d \geq 3$, so that Λ_2 is last. Then there are $4\binom{d}{3}$ minimum cardinality extremal designs of Q_d, each consisting of 2^{d-2} vertices.

Proof. The extremal eigenpolytope in this situation is $P_2 \cong \mathrm{CUT}_d^\square$ and hence it suffices to reason about the facts of $\mathrm{CUT}_d^\square$. Every $\mathrm{CUT}_d^\square$ vertex χ_S corresponds to the pair of Q_d vertices, $\mathbb{1}_S$ and $\mathbb{1}_{[d]\setminus S}$ indexed by a subset S of $[d]$. There are $4\binom{d}{3}$ facets of $\mathrm{CUT}_d^\square$ described by triangle inequalities. By Proposition 2.5.4, these are precisely the facets of $\mathrm{CUT}_d^\square$ with the maximum number of $3 \cdot 2^{d-3}$ vertices.

Fix three distinct indices $i, j, k \in [d]$ and consider the set of vertices of Q_d

$$W = \{\mathbb{1}_S, \mathbb{1}_{[d]\setminus S} : i, j, k \in S\}.$$

Note that there are 2^{d-3} subsets of $[d]$ containing i, j, k. For $\mathbb{1}_S \in W$ and a facet F of $\mathrm{CUT}_d^\square$ defined by the triangle inequality

$$x_{ij} + x_{ik} + x_{jk} \leq 2,$$

$\chi_S \notin F$ since none of the edges ij, ik, or jk are cut: $(\chi_S)_{ij} + (\chi_S)_{ik} + (\chi_S)_{jk} = 0 < 2$. Of the 2^{d-1} vertices of $\mathrm{CUT}_d^\square$, F contains $3 \cdot 2^{d-3}$ vertices and W accounts for 2^{d-3} vertices not on F. Therefore, $\mathbb{1}_S \in W$ with $i, j, k \in S$ if and only if $\chi_S \notin F$. By Theorem 2.3.8, W is a minimum extremal graphical design on Q_d and it has cardinality $2 \cdot 2^{d-3} = 2^{d-2}$.

Likewise, for a facet F defined by the triangle inequality

$$x_{ij} - x_{ik} - x_{jk} \leq 0,$$

$\chi_S \notin F$ if and only if $i, j \in S$ and $k \notin S$. By a similar argument to the one above, the design corresponding to this facet has minimum cardinality and is

$$W' = \{\mathbb{1}_S, \mathbb{1}_{[d]\setminus S} : i, j \in S, k \notin S\}.$$

$\square$

2.5.3 Q_d and the Frequency Order

In the rest of this section we focus on the extremal eigenpolytope (and designs) of Q_d in frequency order. In this order, the last eigenvalue of Q_d is $\lambda_{\frac{d}{2}} = 0$ when d is even and $\lambda_{\frac{d+1}{2}} = -1/d$ or $\lambda_{\frac{d-1}{2}} = 1/d$ when d is odd. These correspond to the "middle" slice(s) of the d-cube. Let m (for "middle") denote the index of the last eigenspace of Q_d in frequency order. Lemma 2.5.1 says the following about P_m.

Lemma 2.5.6. Depending on the parity of d and further, the congruence class of d mod 4, the extremal eigenpolytope of Q_d in frequency order is the following:

1. d even: Then $m = d/2$ and P_m is a polytope of dimension $\binom{d}{\frac{d}{2}}$.

   (a) $d \equiv 0 \bmod 4$: Then P_m is a polytope with 2^{d-1} vertices. Each vertex of P_m comes from two identical columns of U_m given by $c(y) = c(\mathbb{1} - y)$.

   (b) $d \equiv 2 \bmod 4$: Then P_m is a centrally symmetric polytope with 2^d vertices. For each vertex $c(y)$ of P_m, $-c(y) = c(\mathbb{1} - y)$ is also a vertex of P_m.

2. d odd: Then there are two possible indices $m = (d+1)/2$ and $m' = (d-1)/2$ for the extremal eigenpolytopes, and $\dim(P_m) = \binom{d}{\frac{d+1}{2}} = \binom{d}{\frac{d-1}{2}} = \dim(P_{m'})$.

   (a) $d \equiv 1 \bmod 4$: In this case, $m := (d+1)/2$ is odd while $m' := (d-1)/2$ is even. Therefore, P_m is centrally symmetric with 2^d vertices while $P_{m'}$ has 2^{d-1} vertices.

(b) $d \equiv 3 \bmod 4$: In this case $m := (d+1)/2$ is even while $m' := (d-1)/2$ is odd. Therefore, P_m has 2^{d-1} vertices while $P_{m'}$ is centrally symmetric and has 2^d vertices.

Lemma 2.5.6 allows us to upper bound the size of a minimal positively weighted extremal design in Q_d using Theorem 2.3.8.

Corollary 2.5.7. Let W be a minimal positively weighted extremal design in Q_d.

1. If $d \equiv 0 \bmod 4$, then $|W| \leq 2^d - 2\binom{d}{\frac{d}{2}}$.

2. If $d \equiv 1 \bmod 4$, then

$$|W| \leq \min\left\{2^d - 2\binom{d}{\frac{d-1}{2}}, 2^d - \binom{d}{\frac{d+1}{2}}\right\} = 2^d - 2\binom{d}{\frac{d-1}{2}}.$$

3. If $d \equiv 2 \bmod 4$, then $|W| \leq 2^d - \binom{d}{\frac{d}{2}}$.

4. If $d \equiv 3 \bmod 4$, then

$$|W| \leq \min\left\{2^d - 2\binom{d}{\frac{d+1}{2}}, 2^d - \binom{d}{\frac{d-1}{2}}\right\} = 2^d - 2\binom{d}{\frac{d+1}{2}}.$$

Except for $d \equiv 2 \bmod 4$, the upper bounds given in Corollary 2.5.7 are strictly better than those in Theorem 2.3.14 because of the doubling of columns in the matrix U_m. Even so, the bounds in Corollary 2.5.7 are not tight, and we will improve them in the next subsection. For example in Q_5, Corollary 2.5.7 says that there is a positively weighted extremal design of size at most 12 while in fact there is one of size 8. This is because the eigenpolytope P_2 of Q_5 has facets with 12 vertices, each given by two columns of U_2, and so there is an extremal design of size $32 - 24 = 8$. Since $\dim(P_2) = 10$, Corollary 2.5.7 assigns 10 vertices to each facet, each one doubled, so computes $32 - 20 = 12$ as the upper bound. The bound from Theorem 2.3.14 is 22.

2.5.4 Extremal designs and linear codes

By Theorem 2.3.8, the smallest cardinality positively weighted extremal designs in Q_d come from the facets of P_m with the maximum number of vertices. Note that all elements of $\mathcal{U}_m$ are vertices of P_m. Here we use the theory of linear codes to improve the bounds in Corollary 2.5.7.

Definition 2.5.8. Consider the Boolean field $\mathbb{Z}_2 = \{0,1\}$ of integers mod 2 and the $\mathbb{Z}_2$-vector space $\{0,1\}^d$.

1. A *linear code* $C \subseteq \{0,1\}^d$ is a subspace of $\{0,1\}^d$. The *length* of the code C is d and its *dimension* is the dimension of the subspace.

2. The *parity check matrix* of C is a matrix $M \in \{0,1\}^{t\times d}$ such that $C = \ker(M)$.

3. The *dual code* of $C = \ker(M)$ is the linear code $C^\perp := \operatorname{rowspan}(M)$.

We will rely heavily on the following result that connects linear codes to designs.

Lemma 2.5.9 (Theorem 4.8 of [5])**.** Let $C = \ker(M)$ be a linear code in $\{0,1\}^d$. Then C averages the eigenvector φ_x, with $\varphi_x(y) = (-1)^{x^\top y}$, with equal weights if and only if $x \notin C^\perp \setminus \{0\} = \operatorname{rowspan}(M) \setminus \{0\}$.

If the matrix M is chosen so that its row span is contained in the last eigenspace of Q_d in any ordering, then by Lemma 2.5.9, $C = \ker(M)$ would be a combinatorial extremal design in Q_d for that ordering. In fact, by Lemma 2.2.4, both C and its complement in $\{0,1\}^d$ would be combinatorial extremal designs in $\{0,1\}^d$. Equivalently, C partitions the vertices of the extremal eigenpolytope into two faces.

Lemma 2.5.10. The graph Q_d has combinatorial extremal designs for any ordering.

Proof. Let Λ be the last eigenspace of Q_d in a given ordering. Then $\Lambda = \{\varphi_x : |x| = i\}$ for some $i \in [d]$. Choose any $x \in \mathcal{J}_{d,i}$ and consider $W = \ker([x^\top])$. By Lemma 2.5.9, W averages (with equal weights) all eigenspaces of Q_d except Λ. $\square$

This is essentially [43, Theorem 3.3], though that result emphasized that taking any vector as a check matrix provides an extremal design in *some* ordering, and here we emphasize that there is an extremal design for *any* ordering. Using Lemma 2.5.9 it is possible to prove that the minimum cardinality extremal designs in Theorem 2.5.5 are combinatorial.

We now return to frequency ordering and will prove in Theorem 2.5.13 that when $d \equiv 2 \mod 4$, there are positively weighted extremal designs of smallest size that are combinatorial. In the other cases, it is not clear whether the smallest positively weighted extremal designs in Q_d are combinatorial.

Lemma 2.5.11. If i is odd, then the eigenpolytope P_i of Q_d has at least $2\binom{d}{i}$ facets each containing 2^{d-1} vertices. No facet of P_i has more than 2^{d-1} vertices.

Proof. By Lemma 2.5.1, P_i is centrally symmetric. Therefore, the maximum number of vertices that can lie on a single facet of P_i is $2^d/2 = 2^{d-1}$. We will use Gale duality and coding theory to exhibit $\binom{d}{i}$ facets which contain this many vertices. Let $x \in \mathcal{J}_{d,i}$, and consider the parity check matrix $M = [x^\top]$. By Lemma 2.5.9, the code $C = \ker(M)$ averages all eigenspaces of Q_d except for Λ_i. By Theorem 2.3.8, $\{0,1\}^d \setminus C$ are the vertices on a face of P_i. Since the design is combinatorial, C also indexes a face of P_i by Lemma 2.2.4. Since $|C| = 2^{d-1}$, $|\{0,1\}^d \setminus C| = 2^{d-1}$. Therefore, these faces contains the maximum possible number of vertices, and hence must be a facets. There are $\binom{d}{i}$ choices of the vector x. Each provides two unique facets – $\{0,1\}^d \setminus C$ is not a linear code since it does not contain 0. □

The code $\ker(\mathbb{1}^\top)$ is known as the *single parity check code.* Linear codes are said to be equivalent if they only differ by a permutation of coordinates, so the codes $\ker(x^\top)$ are equivalent for any $x \in \mathcal{J}_{d,i}$. In a sense, these codes are generalizations of the single parity check code, but they typically will have poor distance if $x \neq \mathbb{1}$.

If the last eigenspace in frequency order is indexed by an even Hamming weight, then we can always do better.

Lemma 2.5.12. If i is even, then Q_d has a combinatorial design that averages all but Λ_i with strictly fewer than 2^{d-1} vertices.

Proof. Consider a $2 \times d$ check matrix $M = [x_1\ x_2]^\top$ with $x_1, x_2 \in \mathcal{J}_{d,i}$ and $\operatorname{supp} x_1 \cap \operatorname{supp} x_2 = i/2$. This is always possible; here is an example for $d = 9$, $i = 4$:

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}$$

Then, the row span of M is contained in $\mathcal{J}_{d,i}$. By Lemma 2.5.9, $\ker(M)$ averages all eigenspaces of Q_d other than Λ_i, and $|\ker(M)| = 2^{d-2}$. □

We now use the tools we have built so far to find or bound the size of the smallest positively weighted extremal designs in Q_d. Our constructions yield combinatorial designs based on linear codes. We begin by considering the case of $d \equiv 2 \bmod 4$ for which Theorem 2.5.13 provides an optimal answer.

Theorem 2.5.13. Let $d \equiv 2 \mod 4$. A minimum cardinality positively weighted extremal design of Q_d in frequency order consists of 2^{d-1} vertices and is combinatorial. Any code $C = \ker(x^\top)$ for $x \in \mathcal{J}_{d,d/2}$ attains this minimum.

Proof. The last eigenspace of Q_d by frequency is $\Lambda_{d/2}$, and $d/2$ is odd. By Lemma 2.5.11, the extremal eigenpolytope $P_{d/2}$ has facets with 2^{d-1} vertices, the maximum possible, and these vertices are all elements of $\mathcal{U}_{d/2}$. Therefore, a minimum positively weighted extremal design in Q_d consists of 2^{d-1} elements by Theorem 2.3.8. Every linear code of the form $C = \ker(x^\top)$ where $x \in \mathcal{J}_{d,d/2}$ is a combinatorial design that achieves this minimum by Lemma 2.5.9. □

Next we consider $d \not\equiv 2 \mod 4$. In these cases, it follows from Lemmas 2.5.11 and 2.5.12 that when there is a tie for the last eigenspace, the smallest extremal designs are going to come from the extremal eigenpolytope with an even index. Let m be this index in the rest of this section. Concretely,

$$m = \begin{cases} d/2 & \text{if } d \equiv 0 \bmod 4 \\ (d-1)/2 & \text{if } d \equiv 1 \bmod 4 \\ (d+1)/2 & \text{if } d \equiv 3 \bmod 4. \end{cases}$$

We formalize the comments stated after Lemma 2.5.9 for the index m.

Corollary 2.5.14. If the non-zero vectors in the row span of M are entirely of weight m, then the linear code $C = \ker(M)$ is an extremal combinatorial design in Q_d.

Proof. By Lemma 2.5.9, the code C averages all eigenvectors of Q_d except for those indexed by non-zero elements in the row span of M. Since these elements are contained in $\mathcal{J}_{d,m}$, the corresponding eigenvectors all lie in Λ_m. Hence C is an extremal combinatorial design of Q_d. □

Row spans as in Corollary 2.5.14, in which all non-zero elements have the same Hamming weight, are called *linear equidistant codes* or *constant weight linear codes* [13]. These codes have been completely classified by Bonisoli's theorem [16]; we refer the reader also to [105]. We first recall some facts about linear codes. The binary *Hamming code* $H_r \subset \{0,1\}^{2^r-1}$ [86] is the linear code whose check matrix $M_r \in \{0,1\}^{r\times(2^r-1)}$ has columns consisting of the binary expansions of the digits $\{1,\ldots,2^r-1\}$. For instance, the check matrix of $H_3 \subset \{0,1\}^7$ is

$$M_3 = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{bmatrix}.$$

The dual of the Hamming code $H_r^\perp$, i.e., the row span of M_r, is called the *simplex code*, so named because its vectors form the vertex set of a regular (2^r-1)-simplex. Every non-zero element in the simplex code $H_r^\perp$ has weight 2^{r-1}.

Theorem 2.5.15 ([16])**.** If C is a r-dimensional linear equidistant code, then C is equivalent to concatenated copies of the simplex code $H_r^\perp$, possibly with additional zero coordinates.

This means that an r-dimensional linear equidistant code is equivalent to the row span of a maximal concatenation of the check matrix M_r of H_r with possibly additional zero columns. For instance, a 3-dimensional linear equidistant code in $\{0,1\}^{15}$ is equivalent to the row span of $[\ M_3 \mid M_3 \mid \vec{0}\ ]$.

Lemma 2.5.16. For $d \equiv 3 \mod 4$, let $d+1 = 2^t \cdot b$ with t as big as possible. Then t is the maximum dimension of a $((d+1)/2)$-weight linear equidistant code in $\{0,1\}^d$, $\{0,1\}^{d+1}$, and $\{0,1\}^{d+2}$.

Proof. We first show that there are t-dimensional linear equidistant codes of lengths $d, d+1$, and $d+2$. Consider the matrix M given by concatenating b copies of the check matrix M_t. Then $M \in \{0,1\}^{t\times(b(2^t-1))}$. Note that

$$b(2^t - 1) = b2^t - b = d + 1 - b.$$

Since every non-zero element in the row span of M_t has weight 2^{t-1}, every non-zero element in the row span of M has weight

$$b2^{t-1} = (d+1)/2.$$

Thus by appending $b-1$ columns of zeros to M, we arrive at a matrix in $\{0,1\}^{t\times d}$ in which every non-zero element lies in $\mathcal{J}_{d,\frac{d+1}{2}}$. Appending one or two more zero columns creates matrices for which all non-zero elements in their row spans are contained in $\mathcal{J}_{d+1,\frac{d+1}{2}}$ or $\mathcal{J}_{d+2,\frac{d+1}{2}}$, respectively. Note that if $d \equiv 3 \bmod 4$, then $\frac{d+1}{2}$ is even and indexes the extremal eigenspace of interest in Q_d, Q_{d+1} and Q_{d+2}.

We claim that t is the maximum possible dimension of a $((d+1)/2)$-weight linear equidistant code in $\{0,1\}^d$, $\{0,1\}^{d+1}$, and $\{0,1\}^{d+2}$. Let $T > t$, and suppose there is a T-dimensional linear equidistant code of length d and weight $(d+1)/2$. Then this code is the row span of q copies of the Hamming check matrix M_T, possibly padded with some columns of zeros. The weight of each row is $q2^{T-1}$, so $(d+1)/2 = q2^{T-1}$ implies that $d = 2^T q - 1$. Since we also know $d = 2^t b - 1$, it follows that

$$2^T q - 1 = d = 2^t \cdot b - 1 \iff b = 2^{T-t} q$$

Since $T > t$, this implies that b is even, which contradicts the definition of t. A similar argument also works for $d+1$ and $d+2$. $\square$

Theorem 2.5.17. For each triple (d, m, t) shown below, the smallest positively weighted extremal designs of Q_d have at most 2^{d-t} elements and are obtained by choosing Λ_m to be last in frequency order.

1. $d \equiv 0 \bmod 4$: $m = d/2$ and $d = 2^t \cdot b$ with t maximal.

2. $d \equiv 1 \bmod 4$, $m = (d-1)/2$ and $d - 1 = 2^t \cdot b$ with t maximal.

3. $d \equiv 3 \bmod 4$, $m = (d+1)/2$ and $d + 1 = 2^t \cdot b$ with t maximal.

Proof. Note that for each d shown above, the corresponding m in the triple is even and indexes the extremal eigenspace of Q_d (if there is a tie) that can yield the smallest positively weighted designs. This follows from Lemmas 2.5.11 and 2.5.12. By Lemma 2.5.16, there is a maximum cardinality linear equidistant code $C \subset \{0,1\}^d$ of dimension t and weight m. It then follows by the strategy in Corollary 2.5.14 that the dual code $C^\perp$ is then an extremal combinatorial design in Q_d, and $|C^\perp| = 2^{d-t}$. $\square$

We attribute Theorem 2.5.17 to Chris Lee and David Shiroma who discovered these bounds in an undergraduate project supervised by the authors. Following the strategy outlined in Corollary 2.5.14, they discovered the construction in Bonisoli's theorem from which the result follows. Table 2.1 computes the bounds in Theorems 2.5.13 and 2.5.17 for small values of d.

Our main strategy in this chapter has been to use the facet combinatorics of extremal eigenpolytopes to find the smallest positively weighted extremal designs in graphs. In the case of hypercubes, this strategy worked for Q_d when $d \equiv 2 \bmod 4$. In the other cases, it was much harder to understand the facets of the extremal eigenpolytope P_m, and instead we found small designs using the theory of linear codes. By Theorem 2.3.8, these small designs correspond to some faces of the extremal eigenpolytope P_m.

Corollary 2.5.18. In each of the following situations, the extremal eigenpolytope P_m of Q_d has a face containing $2^d - 2^{d-t}$ vertices:

d	m	$\dim(P_m) = \binom{d}{m}$	$\#V(P_m)$	$\|W^*\| \leq$	$\#V(F^*) \geq$
2	1	2	4	2	2
3	2	3	$4 \cdot 2$	2	6
4	2	6	$8 \cdot 2$	4	12
5	2	10	$16 \cdot 2$	8	24
6	3	20	64	32	32
7	4	35	$64 \cdot 2$	16	112
8	4	70	$128 \cdot 2$	32	224
9	4	126	$256 \cdot 2$	64	448
10	5	252	1024	512	512
11	6	462	$1024 \cdot 2$	512	1536

Table 2.1: Bounds from Theorems 2.5.13,2.5.17 for small values of d. W^* denotes a minimum cardinality positively weighted extremal design, and F^* denotes a facet of P_m with the maximum number of vertices including multiplicity. When P_m has N distinct vertices which are doubled up, we write $\#V(P_m) = N \cdot 2$.

1. $d \equiv 0 \bmod 4$, $m = d/2$ $d = 2^t \cdot b$ with t maximal.

2. $d \equiv 1 \bmod 4$, $m = (d-1)/2$ and $d - 1 = 2^t \cdot b$ with t maximal.

3. $d \equiv 3 \bmod 4$, $m = (d+1)/2$ and $d + 1 = 2^t \cdot b$ with t maximal.

Proof. Combinatorial designs are positively weighted designs. Thus the extremal designs of Theorem 2.5.17 provide these faces by Gale duality. $\square$

We conjecture that the bounds in Theorem 2.5.17 are optimal.

Conjecture 2.5.19. The duals of the constant weight codes constructed in Lemma 2.5.16 are smallest cardinality positively weighted extremal designs in their Q_d.

To prove this conjecture, it would suffice to prove the the faces of P_m given by these dual codes are (i) facets of P_m, and (ii) contain the most vertices among all facets of P_m. We note these faces of P_m contain an enormous number of vertices.

We have relied on linear codes to find small designs in Q_d when $d \not\equiv 2 \bmod 4$. However, there is no reason to believe that the smallest, or all minimal, positively weighted extremal designs in such Q_d are codes. Indeed, when $d \not\equiv 2 \bmod 4$, there are minimal positively weighted extremal designs of Q_d that are not isomorphic to linear codes or their complements.

Example 2.5.20. The extremal eigenpolytope P_2 of Q_5 has dimension $10 = \binom{5}{2}$. It has 16 vertices each labeled by two columns of U_2 since $c(y) = c(\mathbb{1} - y)$ for all $y \in \{0,1\}^5$. This polytope has 56 facets that come in two symmetry classes; 16 of them are simplices (Δ_9) each containing $20 = 2 \cdot 10$ columns of U_2 as vertices, while the remaining 40 facets each have $24 = 2 \cdot 12$ vertices. The minimal design complementary to a simplex facet contains $32 - 20 = 12$ vertices of Q_5. A linear code of length 5 must have size 2^t for $t \in [5]$. Since neither 12 nor $32 - 12$ are powers of 2, such a design is not isomorphic to a linear code or its complement.

Chapter 3

EIGENPOLYTOPE UNIVERSALITY AND GRAPHICAL DESIGNS

This chapter is the content of [7], written with David Shiroma, who a student at the University of Washington doing undergraduate research with Rekha Thomas and myself.

3.1 Introduction

This chapter unites two combinatorial constructions arising from the combinatorial graph Laplacian, namely *eigenpolytopes* [40] and *graphical designs* [96], through the theory of *Gale duality* for polytopes [35]. An eigenpolytope is a polytope arising from the eigenspaces of a graph Laplacian. The structure and symmetries of these polytopes provide information about the structure and symmetries of the underlying graph, particularly when the underlying graph is highly structured (see, for instance [42]). A graphical design is a quadrature rule for a graph. Classical numerical quadrature allows one to compute or approximate definite integrals of certain classes of functions on $\mathbb{R}^n$ by sampling at finitely many points. Analogously, a graphical design is a rule to compute the average of certain Laplacian eigenvectors by sampling on a subset of graph vertices. Previous work on graphical designs often focuses on unweighted regular graphs (e.g. [43, 5, 6, 97]), where the eigenvectors of a graph are independent of the choice of graph Laplacian. For regular graphs, the bijection between graphical designs and eigenpolytopes we establish is precisely the one shown in [6]. For more literature review and details on the connection between graphical designs and eigenpolytopes through Gale duality, we refer to [6].

We summarize the main results of this chapter.

- The Laplacian eigenspaces of positively weighted graphs are general: for any collection of orthogonal subspaces which spans $\mathbb{R}^n$ and contains the span of the all-ones vector as a subspace, there exists a connected, positively weighted graph on n vertices whose Laplacian eigenspaces are precisely the given subspaces. The proof reveals a polyhedral structure underlying the possible eigenvalues of a graph with a given eigenbasis. We use this result to prove that every polytope up to affine equivalence appears as an eigenpolytope of a positively weighted graph. Moreover, these algorithms are strongly polynomial time.

- We establish a combinatorial bijection between graphical designs and faces of eigenpolytopes using Gale duality. Polyhedral geometry then provides an upper bound on the size of the support of minimal graphical designs. We note that this bijection holds when the combinatorial Laplacian is replaced by any symmetric operator with the all-ones vector as an eigenvector.

- Through Gale duality and our algorithms, we establish complexity results for graphical designs as translations of polytope hardness results. We provide a linear program which finds a graphical design in polynomial time with a guaranteed sparseness, though minimality is not guaranteed.

We organize the chapter as follows. Section 3.2 introduces eigenpolytopes. Section 3.3 contains our algorithmic results showing the universality of Laplacian eigenspaces and eigenpolytopes. Section 3.4 establishes definitions and notation for graphical designs on positively weighted graphs. Section 3.5 briefly recounts the theory of Gale duality for polytopes and uses this machinery to connect graphical designs to the eigenpolytopes of the graph, a key structural result. This correspondence provides a proof of existence and an upper bound on the size of a minimal graphical design. Using our strongly polynomial time algorithms to create graphs with given eigenpolytopes, we establish the following complexity results in Section 3.6 by translating established hardness results for polytopes. It is strongly NP-complete to determine if there is a design smaller than the upper bound established in Section 3.5, it is NP-hard to find a smallest graphical design, and it is #P-complete to count the number of support-minimal graphical designs.

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3.2 Eigenpolytopes of Weighted Graphs

Let $G = ([n], E, w)$ be a connected graph with vertex set $[n] := \{1, 2, \ldots, n\}$, edge set E, and positive edge weights $w : E \to \mathbb{R}_{>0}$. Let $A \in \mathbb{R}^{n\times n}$ be the weighted adjacency matrix of G, with $A_{ij} = w(ij)$ if $ij \in E$ and 0 otherwise, and D be the weighted (diagonal) degree matrix of G, with $D_{ii} = \deg i = \sum_{ij\in E} w(ij)$. The (combinatorial) Laplacian of G is the symmetric matrix $L = D - A$. Since L is positive semidefinite, it has non-negative eigenvalues and an orthogonal set of eigenvectors $\phi_1, \ldots, \phi_n$ that form a basis of $\mathbb{R}^n$.

Letting $\mathbb{1}$ denote the all-ones vector in $\mathbb{R}^n$, we always have that $L\mathbb{1} = 0$, since the i-th row of A sums to $\deg(i) = \sum_{ij\in E} w(ij)$. Therefore, $\mathbb{1}$ is an eigenvector of L with eigenvalue 0. Moreover, since G is connected, the eigenspace of 0 is spanned by $\mathbb{1}$; we denote this eigenspace by Λ_1. It is convenient to not normalize the eigenvectors ϕ_i so that we may take $\varphi_1 = \mathbb{1}$ as the basis vector for Λ_1. We refer to the eigenspaces and eigenvalues of L as the eigenspaces and eigenvalues of the graph G. We use the following running example to illustrate many definitions and results. The circled numbers in a graph are a labeling of the graph vertices.

Example 3.2.1. Consider the weighted graph in Figure 3.1. The weights are given by $w(ij) = 1/|N(i)| + 1/|N(j)|$, where $|N(i)|$ is the number of edges incident to i.

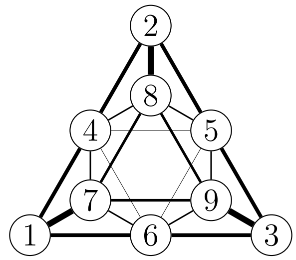


Figure 3.1: A weighted graph on nine vertices. Thicker edges indicate greater edge weights.

Its Laplacian L is

$$1/30 \begin{bmatrix} 46 & 0 & 0 & -15 & 0 & -15 & -16 & 0 & 0 \\ 0 & 46 & 0 & -15 & -15 & 0 & 0 & -16 & 0 \\ 0 & 0 & 46 & 0 & -15 & -15 & 0 & 0 & -16 \\ -15 & -15 & 0 & 72 & -10 & -10 & -10 & -10 & 0 \\ 0 & -15 & -15 & -10 & 72 & -10 & 0 & -11 & -11 \\ -15 & 0 & -15 & -10 & -10 & 72 & -11 & 0 & -11 \\ -16 & 0 & 0 & -11 & 0 & -11 & 62 & -12 & -12 \\ 0 & -16 & 0 & -11 & -11 & 0 & -12 & 62 & -12 \\ 0 & 0 & -16 & 0 & -11 & -11 & -12 & -12 & 62 \end{bmatrix}.$$

Table 3.1 shows the six distinct eigenvalues of L in the left column, each followed on the right by a basis of orthogonal eigenvectors for that eigenspace. We note that $\lambda_2, \lambda_4, \lambda_6$ are the roots of $450x^3 - 3030x^2 + 6321x - 3844$ and λ_3, λ_5 are the roots of $75x^2 - 340x + 373$. We show decimal approximations for conciseness.

For a given graph G with m eigenspaces, we denote a fixed arbitrary ordering of the eigenspaces as $\Lambda_1 = \text{span}\{\mathbb{1}\} < \ldots < \Lambda_m$. Let U denote a matrix whose rows are an eigenbasis of L, and let $I \subset [m]$ index a proper subset of eigenspaces of G. We use U_I to denote the submatrix of U consisting of all rows corresponding to the eigenspaces Λ_i for $i \in I$. Let $\mathcal{U}_I$ denote the collection of columns of U_I, which we note may occur with repetition.

vertex	1	2	3	4	5	6	7	8	9
$\lambda_1 = 0$	1	1	1	1	1	1	1	1	1
$\lambda_2 = 1.069$	−.6262	.5616	.0646	−.0264	.256	−.2291	−.3059	.2744	.0316
	−.2870	−.3988	.6858	−.2798	.1171	.1627	−.1402	−.1948	.3350
$\lambda_3 = 1.861$	.3193	.3193	.3193	.1406	.1406	.1406	−.4600	−.4600	−.4600
$\lambda_4 = 2.661$	.3248	−.4014	.0766	.0507	.2150	−.2658	−.4852	.5996	−.1144
	.2760	.1433	−.4193	−.2776	.1827	.0949	−.4123	−.2141	.6263
$\lambda_5 = 2.672$	.3468	.3458	.3468	−.4499	−.4499	−.4499	.1032	.1032	.1032
$\lambda_6 = 3.003$	.0724	−.0995	.0271	.1880	.5015	−.6894	.2707	−.3721	.1015
	.0731	.0261	−.0992	−.6876	.5066	.1810	.2734	.0977	−.3711

Table 3.1: The spectral information of the graph shown in Figure 3.1.

Definition 3.2.2. Let $G = ([n], E, w)$ have m eigenspaces $\Lambda_1 < \ldots < \Lambda_m$, and let $I \subset [m]$ index a set of eigenvalues of G. The polytope $P_I = \mathrm{conv}(\mathcal{U}_I)$ is a (Laplacian) *eigenpolytope* of G for the eigenvalues indexed by I.

Example 3.2.3. Figure 3.2 shows the eigenpolytope $P_{\{5,6\}}$ of the graph G from Example 3.2.1, using the same eigenspace ordering as in Table 3.1. Its vertices are given by the columns of the following submatrix extracted from Table 3.1, where the horizontal line separates Λ_5 from Λ_6.

$$\left[\begin{array}{ccccccccc} .3468 & .3458 & .3468 & -.4499 & -.4499 & -.4499 & .1032 & .1032 & .1032 \\ \hline .0724 & -.0995 & .0271 & .1880 & .5015 & -.6894 & .2707 & -.3721 & .1015 \\ .0731 & .0261 & -.0992 & -.6876 & .5066 & .1810 & .2734 & .0977 & -.3711 \end{array}\right]$$

Eigenpolytopes were first defined by Godsil in [40] for single eigenspaces of the adjacency matrix A. The eigenpolytopes P_I are more general in the sense that they correspond to multiple eigenvalues of L and allow for weighted graphs. Though the definition depends on a choice of eigenbasis, eigenpolytopes of a graph are well defined up to affine equivalence, which is sufficient for our purposes.

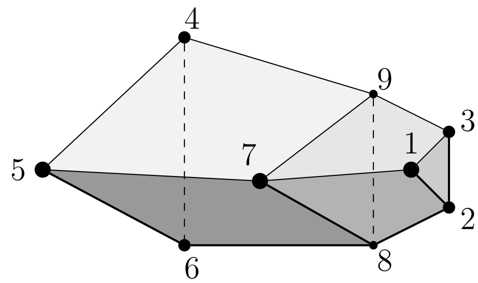


Figure 3.2: The eigenpolytope $P_{\{5,6\}}$ of the running example

3.3 Weighted Graphs From Polytopes

In this section, we show that any polytope up to affine equivalence can appear as an eigenpolytope of a positively weighted graph. We first show that any orthogonal basis for $\mathbb{R}^n$ which includes $\mathbb{1}$ as a basis vector, and any partition of this basis with $\{\mathbb{1}\}$ as a part, give rise to a positively weighted graph $G = ([n], E, w)$ where each part of the partition spans a distinct Laplacian eigenspace of G. Our proof reveals a polyhedral structure underlying the valid choices of eigenvalues that define such graphs. These results are phrased in terms of rational numbers for the purpose of time-complexity statements, but the same algorithms are valid for real numbers.

The *size* of a rational number $r = p/q$ in reduced form is

$$\operatorname{size}(r) = 1 + \lceil \log_2(|p| + 1) \rceil + \lceil \log_2(|q| + 1) \rceil,$$

and the *size* of a rational matrix $B \in \mathbb{Q}^{n \times m}$ is

$$\operatorname{size}(B) = mn + \sum_{i,j} \operatorname{size}(B_{ij}).$$

An algorithm is *strongly polynomial time* if its run time is polynomial in size of the input, not just the dimension of the input.

We overload the notation Diag; for a vector $v \in \mathbb{R}^n$, $\operatorname{Diag}(v) \in \mathbb{R}^{n \times n}$ is the diagonal matrix with $\operatorname{Diag}(v)_{ii} = v_i$, and for a matrix $M \in \mathbb{R}^{n \times n}$, $\operatorname{Diag}(M) \in \mathbb{R}^{n \times n}$ is the diagonal matrix which forgets the off-diagonal entries of M.

Lemma 3.3.1. Let $\mathcal{B} = \{\varphi_1 = \mathbb{1}, \varphi_2, \ldots, \varphi_n\}$ be a rational orthogonal basis of $\mathbb{R}^n$, partitioned as $\mathcal{B} = \pi_1 \sqcup \ldots \sqcup \pi_m$ with at least two parts such that $\pi_1 = \{\mathbb{1}\}$. There is a connected graph G with positive rational edge weights and m Laplacian eigenspaces $\Lambda_1, \ldots, \Lambda_m$ such that π_i spans Λ_i. The graph G can be constructed in strongly polynomial time.

Proof. Let $B \in \mathbb{Q}^{n\times n}$ have i-th row φ_i. Then the rows of $\tilde{B} = \mathrm{Diag}(\frac{1}{\|\varphi_1\|}, \ldots, \frac{1}{\|\varphi_n\|})B$ form an orthonormal basis of $\mathbb{R}^n$. We seek a rational matrix $M = \mathrm{Diag}(0, \lambda_2, \ldots, \lambda_n)$ with $\lambda_i > 0$ and $\lambda_i = \lambda_j$ if and only if φ_i and φ_j lie in the same part of the partition so that $L = \tilde{B}^\top M \tilde{B}$ is the Laplacian of a positively weighted graph.

Assuming such an M exists, $A = \mathrm{Diag}(\tilde{B}^\top M \tilde{B}) - \tilde{B}^\top M \tilde{B}$ is then the adjacency matrix of the desired graph G, which has Laplacian eigenspaces $\Lambda_1, \ldots, \Lambda_m$ where Λ_i is spanned by π_i. We first check several properties of this construction.

1. L is positive semidefinite: We see that $L = (M^{1/2}\tilde{B})^\top (M^{1/2}\tilde{B})$.

2. $D = \mathrm{Diag}(\tilde{B}^\top M \tilde{B})$ is the degree matrix of G: Since $\tilde{B}^\top M \tilde{B}\mathbb{1} = 0$, D satisfies $D_{ii} = (\tilde{B}^\top M \tilde{B})_{ii} = -\sum_{j\neq i} (\tilde{B}^\top M \tilde{B})_{ij} = \sum_{j \neq i} A_{ij} = \deg(i)$.

3. G is connected: By construction, the multiplicity of 0 as an eigenvalue is 1.

4. G has rational weights. For $i \neq j$,

$$w_{ij} = -L_{ij} = -\sum_{k=2}^{n} \frac{\varphi_k(i)\varphi_k(j)\lambda_k}{\varphi_k^\top \varphi_k} \in \mathbb{Q}$$

5. It is strongly polynomial time to compute A from B and M. The most expensive operation is multiplication of $n \times n$ matrices.

It remains to show that we can find an M with the given properties so that $A \geq 0$. For the rest of this proof, let $\mathbb{1} \in \mathbb{R}^{n-1}$. We will prove that such an M exists by showing that $M = \mathrm{Diag}(0, \mathbb{1}^\top)$ lies in the interior of the constraints imposed by $A \geq 0$, and can be perturbed to satisfy all the needed conditions. We note that $M = \mathrm{Diag}(0, \mathbb{1}^\top)$ corresponds to an equally weighted complete graph and solves the problem when $m = 2$. Since $\lambda_1 = 0$,

$$L = \tilde{B}^\top M \tilde{B} = \sum_{k=1}^{n} \frac{\lambda_k}{\|\varphi_k\|^2} \varphi_k \varphi_k^\top = \sum_{k=2}^{n} \frac{\lambda_k}{\|\varphi_k\|^2} \varphi_k \varphi_k^\top .$$

Since we require positive edge weights, we need that for $i \neq j$,

$$A_{ij} = -L_{ij} = -\sum_{k=2}^{n} \frac{\varphi_k(i)\varphi_k(j)\lambda_k}{\|\varphi_k\|^2} \geq 0.$$

This provides a system of $n(n-1)/2$ linear inequalities constraining the choice of eigenvalues. Represent this system as $C\lambda \geq 0$, where $\lambda = (\lambda_2, \dots, \lambda_n) \in \mathbb{R}^{n-1}$ and $C \in \mathbb{R}^{n(n-1)/2 \times (n-1)}$. We note that $K = \{\lambda \in \mathbb{R}_+^{n-1} : C\lambda \geq 0\}$ is a polyhedral cone. For some $i \neq j$, let

$$c = \left(\frac{-\varphi_2(i)\varphi_2(j)}{\|\varphi_2\|^2}, \dots, \frac{-\varphi_n(i)\varphi_n(j)}{\|\varphi_n\|^2} \right)^\top$$

be a row of C. Since $\tilde{B}$ is orthonormal, the columns of $\tilde{B}$ are orthogonal. Therefore,

$$\begin{aligned} 0 &= \left(\frac{1}{\sqrt{n}}, \frac{\varphi_2(i)}{\|\varphi_2\|}, \cdots, \frac{\varphi_n(i)}{\|\varphi_n\|} \right) \left(\frac{1}{\sqrt{n}}, \frac{\varphi_2(j)}{\|\varphi_2\|}, \cdots, \frac{\varphi_n(j)}{\|\varphi_n\|} \right)^\top \\ &= \frac{1}{n} + \sum_{k=2}^{n} \frac{\varphi_k(i)\varphi_k(j)}{\|\varphi_k\|^2} = \frac{1}{n} - c^\top \mathbb{1}. \end{aligned}$$

Hence $c^\top \mathbb{1} = \frac{1}{n} > 0$. Since c was an arbitrary row of C, we see that $C\mathbb{1} > 0$, implying that the ray spanned by $\mathbb{1}$ lies in the interior of K. Thus there is an ε-neighborhood of $\mathbb{1}$

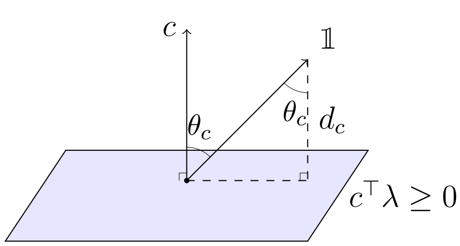


Figure 3.3: Computing the distance from $\mathbb{1}$ to ∂K

contained in K. Let θ_c be the angle between $\mathbb{1}$ and c. Observe from Figure 3.3 that the distance between $\mathbb{1}$ and the hyperplane $c^\top \lambda \geq 0$ is

$$d_c = \|\mathbb{1}\| \cos\theta_c = \|\mathbb{1}\| \cdot \frac{c^\top \mathbb{1}}{\|c\|\|\mathbb{1}\|} = \frac{1}{n\|c\|} > 0.$$

Then such $\varepsilon \in \mathbb{Q}$ can be computed in strongly polynomial time by rounding down each d_c to two significant digits, taking the minimum over all possible d_c's, and multiplying by some constant $\alpha < 1$ (e.g. $\alpha = 0.99$). For $k = 2, \dots, n$, if $\varphi_j \in \pi_k$, define $\lambda_j := 1 + \delta_j$, where $\delta_j = \frac{\widetilde{k}\varepsilon}{n}$ and $\widetilde{k}$ is a rational approximation of $\sqrt{k}$ up to the precision needed to distinguish $\sqrt{m-1}$ from $\sqrt{m}$. Finding such an approximation takes time $\mathcal{O}(\log(m) + \text{precision})$ using binary search, and the precision depends polynomially on $m < n$. Note that $\sum_{k=2}^{m} |\pi_k| = |\mathcal{B}| - 1 = n - 1$. Then,

$$\|\lambda - \mathbb{1}\| \leq \frac{\varepsilon}{n} \left(\sum_{k=2}^{m} k|\pi_k| \right)^{\frac{1}{2}} \leq \frac{\varepsilon}{n} \left(n \sum_{k=2}^{m} |\pi_k| \right)^{\frac{1}{2}} = \frac{\varepsilon}{n} \left(n(n-1)\right)^{\frac{1}{2}} < \varepsilon.$$

By construction, $\lambda > 0$ since it is in the ε-neighborhood of $\mathbb{1}$, and $\lambda \in \mathbb{Q}^{n-1}$ satisfies the requirements imposed by the given eigenspace partition. Thus we have found the desired matrix $M = \mathrm{Diag}(0, \lambda_2, \dots, \lambda_n) \in \mathbb{Q}^{n \times n}$. $\square$

For a given orthogonal basis $\mathcal{B}$, the cone

$$K = \{\lambda = (\lambda_2, \dots, \lambda_n) \geq 0 : C\lambda \geq 0\}$$

in the proof of Lemma 3.3.1 indexes all possible positively weighted graphs with $\mathcal{B}$ as its eigenvectors. The graph defined by λ is missing edges if and only if λ is in the boundary of K, and the facial structure of K indexes the possible sparsity patterns of positively weighted graphs with these eigenvectors.

Furthermore, the braid arrangement partitions K into chambers corresponding to the order of eigenvalues, which we depict for $n = 4$ in Figure 3.4. Using nonstandard notation to be compatible with the notation of K, recall that the braid arrangement in $\mathbb{R}^n$ is the collection of hyperplanes

$$\mathcal{A}_n = \{H_{ij} = \{\lambda = (\lambda_2, \dots, \lambda_{n+1}) : \lambda_i = \lambda_j\}\}_{2=i<j\leq n+1}.$$

Points lying on H_{ij} correspond to graphs where the eigenspaces collapse into each other. As more hyperplanes of $\mathcal{A}_n$ intersect, an eigenvalue has higher multiplicity.

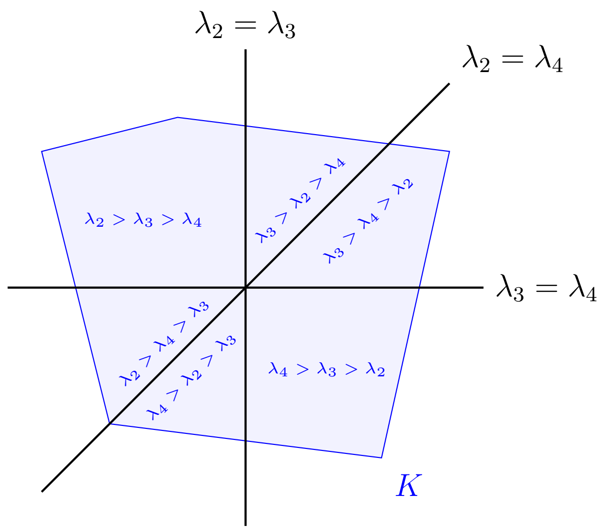


Figure 3.4: A cross-section of the braid arrangement $\mathcal{A}_3$ intersecting the cone K of eigenvalues. The center point corresponds to $\lambda = \mathbb{1}$, which defines the unweighted complete graph.

We now use Lemma 3.3.1 to show that given a polytope P, we can construct a positively weighted graph in strongly polynomial time which has an eigenpolytope that is affinely equivalent to P.

Theorem 3.3.2. Let $\mathcal{V} = \{v_1, \ldots, v_n\} \subset \mathbb{Q}^d$, and let $P = \operatorname{conv}(\mathcal{V})$ be full dimensional. We can create a connected graph $G = ([n], E, w)$ with $w \in \mathbb{Q}^E_{>0}$ which has a Laplacian eigenpolytope that is affinely equivalent to P in strongly polynomial time.

Proof. We may translate P so that its centroid lies at the origin by mapping $v_i \mapsto v_i - \frac{1}{n}\sum_{i=1}^n v_i$. This is an affine transformation, and

$$\sum_{i=1}^{n}\left(v_i - \frac{1}{n}\sum_{i=1}^{n} v_i\right) = \sum_{i=1}^{n} v_i - n\frac{1}{n}\sum_{i=1}^{n} v_i = 0.$$

Thus, we may assume without loss of generality that $\sum_{i=1}^n v_i = 0$, or equivalently, that the rows of the matrix $V = [v_1 \ldots v_n]$ are orthogonal to $\mathbb{1}$. Let $X = [x_1 \, \ldots \, x_n] \in \mathbb{Q}^{(n-d-1)\times n}$ have rows which form a basis for the kernel of the matrix $[\mathbb{1}\ V^\top]^\top$. We can find X in strongly polynomial time using Gaussian elimination (see [89, Theorem 23.3]). Let

$$\hat{B} = \begin{bmatrix} \mathbb{1}^\top \\ V \\ X \end{bmatrix}.$$

We will think of the rows of $\hat{B}$ as the Laplacian eigenvectors of the graph we will construct. Perform Gram-Schmidt orthogonalization on the rows of $\hat{B}$ to obtain a rational orthogonal matrix

$$B = \begin{bmatrix} \mathbb{1} & \varphi_2 & \dots & \varphi_n \end{bmatrix}^\top.$$

Gram-Schmidt orthogonalization is a subroutine of the LLL algorithm [60] which is strongly polynomial (see [89, Corollary 6.4a]), hence Gram-Schmidt is strongly polynomial. Note that $\operatorname{span}\{\varphi_2, \dots, \varphi_{d+1}\} = \operatorname{rowspan} V$ because Gram-Schmidt sequentially preserves span. By Lemma 3.3.1, we can construct a graph with rational, positive edge weights with the following three eigenspaces in strongly polynomial time: $\Lambda_1 = \operatorname{span}\{\mathbb{1}\}, \Lambda_2 = \operatorname{span}\{\varphi_2, \dots, \varphi_{d+1}\}, \Lambda_3 = \operatorname{span}\{\varphi_{d+2}, \dots, \varphi_n\}$. Because V and $[\varphi_2 \dots, \varphi_{d+1}]^\top$ differ only by a change of basis, the eigenpolytope $P_{\{2\}}$ is affinely equivalent to $P = \operatorname{conv}(\mathcal{V})$. $\square$

Corollary 3.3.3. Up to affine equivalence, every polytope with n vertices appears as the eigenpolytope of a positively weighted graph on n vertices.

Example 3.3.4. We illustrate Theorem 3.3.2 by embedding the 16-cell, also known as the 4-dimensional cross polytope, as the eigenpolytope of a connected, positively weighted graph. A centered, orthogonal embedding of the 16-cell's vertices is

$$V = \begin{bmatrix} 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \end{bmatrix}.$$

We next compute an orthogonal basis for the kernel of $[\mathbb{1}, V^\top]^\top$:

$$X = \begin{bmatrix} -1 & 1 & 0 & 0 & -1 & 1 & 0 & 0 \\ -1 & -1 & 2 & 0 & -1 & -1 & 2 & 0 \\ -1 & -1 & -1 & 3 & -1 & -1 & -1 & 3 \end{bmatrix}.$$

We set the eigenspace partition $\Lambda_1 = \operatorname{span}\{\mathbb{1}\}, \Lambda_2 = \operatorname{rowspan} V, \Lambda_3 = \operatorname{rowspan} X$. Following the procedure in Lemma 3.3.1, we compute the following cone of eigenvalues for which the resulting graph will be positively weighted.

$$K = \left\{ (\lambda_2, \lambda_3) : \begin{bmatrix} 0 & 1/8 \\ 1/2 & -3/8 \end{bmatrix} \begin{bmatrix} \lambda_2 \\ \lambda_3 \end{bmatrix} \geq 0 \right\}$$

A valid choice of eigenvalues is $\lambda_2 = 20$, $\lambda_3 = 24$. We depict the resulting complete weighted graph in Figure 3.5.

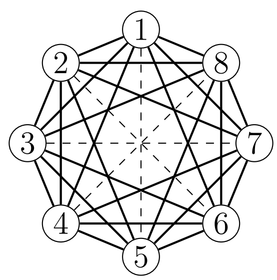


Figure 3.5: A graph which has the 16-cell as an eigenpolytope. Solid edges have weight 3, dashed edges have weight 1.

Our embedding of a polytope as an eigenpolytope uses eigenvalues from the interior of the cone K, so the resulting graph will always be dense. To find a non-complete graph with the given eigenpolytope, one needs to find eigenvalues lying in the boundary of the cone K. We will use this idea to show that the edge graph of the 16-cell has the 16-cell as an eigenpolytope, a result due to [42, Theorem 4.3]. The first inequality of K ($\lambda_3/8 \geq 0$) cannot hold at equality without disconnecting the graph. However, $\lambda_2/2 - 3\lambda_3/8 = 0$ has positive

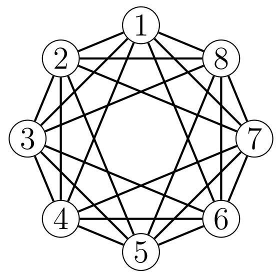


Figure 3.6: The graph of the 16-cell, for which the 16-cell is an eigenpolytope.

solutions, and

$$\begin{bmatrix} 0 & 1/8 \\ 1/2 & -3/8 \end{bmatrix} \begin{bmatrix} 6 \\ 8 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

shows that $(6, 8) \in K$. Thus the graph defined by the Laplacian

$$L = \begin{bmatrix} \mathbb{1} & V^\top & X^\top \end{bmatrix} \operatorname{Diag}(0, 6, 6, 6, 6, 8, 8, 8) \begin{bmatrix} \mathbb{1}^\top \\ V \\ X \end{bmatrix}^{-1}$$

is not dense and has the 16-cell as an eigenpolytope. Working out the computations shows that this graph is truly the graph of the 16-cell, depicted in Figure 3.6.

We show in Example 3.3.5 that not every polytope may be embedded as the eigenpolytope of an unweighted graph on n vertices. The flexibility to use positive edge weights is crucial for this universality result.

Example 3.3.5. Up to affine equivalence, the quadrilateral

$$P = \operatorname{conv} \left\{ \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 2 \end{bmatrix} \right\}$$

is not an eigenpolytope of any unweighted graph with four vertices. Following the procedure of Theorem 3.3.2, we find the following orthogonal basis of $\mathbb{R}^4$, where the middle two rows correspond to the polytope:

$$B = \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ \hline -1 & -1 & 1 & 1 \\ -1 & 1 & -2 & 2 \\ \hline 2 & -2 & -1 & 1 \end{array}\right].$$

Following Lemma 3.3.1, any graph with this polytope as an eigenpolytope has

$$L = B^\top \operatorname{Diag}(1/2, 1/2, 1/10, 1/10) \operatorname{Diag}(0, a, b, c)B,$$

where $a, b, c > 0$ and $a, b \neq c$, but we allow the possibility of $a = b$. Unraveling the multiplication, four unique expressions describe the edge weights of this graph.

$a/4 - b/10 - 2c/5$	edge $(1, 2)$
$-a/4 + b/5 - c/5$	edges $(1, 3), (2, 4)$
$-a/4 - b/5 + c/5$	edges $(1, 4), (2, 3)$
$a/4 - 2b/5 - c/10$	edge $(3, 4)$

We check using MATLAB[68] that for each $v \in \{0, -1\}^4$, the linear system

$$\begin{bmatrix} 1/4 & -1/10 & -2/5 \\ -1/4 & 1/5 & -1/5 \\ -1/4 & -1/5 & 1/5 \\ 1/4 & -2/5 & -1/10 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = v$$

is either inconsistent or forces $b = c$. Thus no unweighted graph has an eigenpolytope which is affinely equivalent to this polytope.

To end this section, we contrast Theorem 3.3.2 with related results on Colin de Verdière matrices ([26], see also [104]). A Colin de Verdière matrix for an unweighted graph $G = ([n], E)$ is any matrix of the form $M = \delta - \hat{A}$, where

1. $\hat{A}$ is the weighted adjacency matrix of a positively weighted graph $\hat{G} = ([n], E, w)$ on the same edge set as G,

2. δ is an arbitrary diagonal matrix, and

3. M has exactly one negative eigenvalue.

By definition, M is not positive semidefinite and need not have row sums equal to one. For our purposes, we can think of these matrices as something like a Laplacian on a graph with not only positive edge weights, but also (arbitrary) vertex weights. Lovász and Schrijver show in [65] that any 3-dimensional polytope is an eigenpolytope of its edge graph for every Colin de Verdière matrix with corank three. Izmestiev extends this construction in [52] to show that every polytope is an eigenpolytope of its edge graph for a specifically constructed Colin de Verdière matrix. These universality results for eigenpolytopes of Colin de Verdière matrices guarantee a serious amount of sparsity in the graphs needed to represent a given polytope as an eigenpolytope. We note, however, that M is not exactly a Laplacian, and the underlying graph has arbitrary vertex weights. To find the specific Colin de Verdière matrix in Izmestiev's construction requires computing the volume of a polytope, which is a #P-hard problem [31]. Our construction generally produces a dense graph, but we do not require vertex weights, the matrix we use is the true combinatorial graph Laplacian, and the algorithm is strongly polynomial time.

3.4 Graphical Designs

A graphical design on $G = ([n], E, w)$ is a proper subset of graph vertices $S \subset [n]$ on which the global averages of certain graph eigenvectors agree with the weighted averages over just the subset S. If φ is such an eigenvector, that means we seek $S \subset [n]$ and quadrature weights $a_s \in \mathbb{R}$, $s \in S$ such that

$$\frac{1}{n}\sum_{i=1}^{n}\varphi(i) = \sum_{s\in S} a_s\varphi(s).$$

The support of a vector $a \in \mathbb{R}^n$ is $\operatorname{supp}(a) := \{i \in [n] : a_i \neq 0\}$. A graphical design S with weights a_s may be identified with the vector $a \in \mathbb{R}^n$ where $S = \operatorname{supp}(a)$. We gloss over some motivation and explanation for the formal definition in Definition 3.4.1. We refer those seeking more detail to [6], where a nearly identical story is developed for regular unweighted graphs using the Laplacian AD^{-1}.

We recall our previous notation and establish some more. For a given graph G with m eigenspaces, we denote a fixed arbitrary ordering of the eigenspaces as $\Lambda_1 = \text{span}\{\mathbb{1}\} < \ldots < \Lambda_m$. The rows of the matrix U form an eigenbasis of L, and for $I \subset [m]$, we use U_I to denote the submatrix of U consisting of all rows corresponding to the eigenspaces Λ_i for $i \in I$. Lastly, $\mathcal{U}_I$ denotes the collection of columns of U_I. We use $\boldsymbol{k}$ to denote the particular index set $\{2, \ldots, k\} \subset [m]$. For a subset $S \subset [n]$, define $\mathbb{1}_S$ by $\mathbb{1}_S(i) = 1$ if $i \in S$ and 0 otherwise.

Definition 3.4.1 (k-graphical designs)**.** Suppose $G = ([n], E, w)$ has eigenspaces $\Lambda_1 = \text{span}\{\mathbb{1}\} < \ldots < \Lambda_m$.

1. A *weighted k-graphical design* of G is a subset $S \subset [n]$ and real weights $(a_s \neq 0 : s \in S)$ such that $U_{\boldsymbol{k}} a = 0$.

2. If additionally $a \geq 0$, we call S a *positively weighted k-graphical design*.

3. If $a = \mathbb{1}_S$ then S is a *combinatorial k-graphical design*.

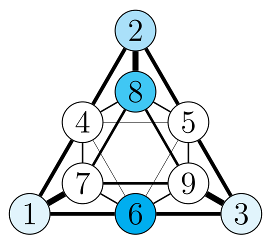
We only consider graphical designs up to scaling. If $U_{\boldsymbol{k}} a = 0$, then any scaling of a is also in the kernel of $U_{\boldsymbol{k}}$. For this reason we leave Λ_1 out of the definition, as any vector a can be scaled to average this eigenspace. We also note that no proper subset is an m-graphical design – this follows by the same argument as in [6, Lemma 2.5]. Though $\mathbb{1}$ is always a k-graphical design for all $k \in [m]$, the purpose of a graphical design is, in a sense, to compress data on a graph, so we restrict our attention to proper subsets of graph vertices.

We will often abbreviate k-graphical designs as k-designs. We note that there are two kinds of weights at play in our setup: the edge weights w of the graph, and the quadrature weights a_s which define the design. Here, we will only consider positively weighted or combinatorial designs. Quadrature rules with negative weights are typically undesirable, as they can lead to nonconvergence and instability [51].

Example 3.4.2. Consider the graph from Example 3.2.1 shown in Figure 3.1 with eigenspaces ordered as labeled. The quadrature weights

$$a_1 = a_3 = .0342,\ a_2 = .1111,\ a_6 = .5328,\ a_8 = .2876,$$

show that $S = \{1, 2, 3, 6, 8\}$ averages the basis vectors given for $\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_4$, which is to say that $U_{\{2,3,4\}}a = 0$. Thus these vertices with these weights form a positively weighted 4-graphical design, shown in Figure 3.7 along with the full matrix $U_{\{2,3,4\}}$. In this ordering of the eigenspaces, there are no combinatorial 4-designs.



$$\begin{bmatrix} -.6262 & .5616 & .0646 & -.0264 & .2560 & -.2291 & -.3059 & .2744 & .0316 \\ -.2870 & -.3988 & .6858 & -.2798 & .1171 & .1627 & -.1402 & -.1948 & .3350 \\ .3193 & .3193 & .3193 & .1406 & .1406 & .1406 & -.4600 & -.4600 & -.4600 \\ .3248 & -.4014 & .0766 & .0507 & .2150 & -.2658 & -.4852 & .5996 & -.1144 \\ .2760 & .1433 & -.4193 & -.2776 & .1827 & .0949 & -.4123 & -.2141 & .6263 \end{bmatrix}$$

Figure 3.7: A positively weighted 4-graphical design on a positively weighted graph. A more saturated color on a vertex indicates a larger vertex weight in the design. The matrix $U_{\{2,3,4\}}$ is also shown, with the relevant columns highlighted in cyan.

3.5 A Bijection through Gale Duality

We now use Gale duality to connect graphical designs and eigenpolytopes, extending the results in [6] for unweighted regular graphs to positively weighted graphs without regularity assumptions. We begin with a brief introduction to Gale duality, due to [35]; see [109, 45] for more details.

A *vector configuration* $\mathcal{V} = (v_1, \ldots, v_n)$ is a collection of real vectors with possible repetitions. We denote the matrix $[v_1 \ \ldots \ v_n]$ by V. A *dependence* on $\mathcal{V}$ is a vector $a \in \mathbb{R}^n$ such that $Va = 0$. A support-minimal dependence is called a *circuit* of $\mathcal{V}$.

Theorem 3.5.1 (Gale Duality)**.** Suppose

$$\mathcal{V} = (v_1, \ldots, v_n),\ v_i \in \mathbb{R}^{n-d-1} \text{ and } \mathcal{V}^* = (v_1^*, \ldots, v_n^*),\ v_i^* \in \mathbb{R}^{d+1}$$

are vector configurations satisfying the following properties.

1. V and V^* are full rank matrices.

2. $V(V^*)^\top = 0$

3. $\mathbb{1}$ is the first row of V^*.

Then, for any $I \subseteq [n]$, $\text{conv}\{v_i^* : i \in [n] \setminus I\}$ is a face of $P^* = \text{conv}(\mathcal{V}^*)$ if and only if 0 is in the relative interior of $\text{conv}\{v_i : i \in I\}$.

For an index set $I \subseteq [n]$, 0 is in the relative interior of $\text{conv}\{v_i : i \in I\}$ if and only if there exists $c \geq 0$ with $\text{supp}(c) = I$ and $Vc = 0$. Equivalently c is a positive dependence of $\mathcal{V}$ with $\text{supp}(c) = I$. Therefore we have the following consequence.

Corollary 3.5.2. Let $\mathcal{V}$ and $\mathcal{V}^*$ be as in Theorem 3.5.1. For any $I \subseteq [n]$, $\text{conv}\{v_i^* : i \in [n] \backslash I\}$ is a face (facet) of $P^* = \text{conv}(\mathcal{V}^*)$ if and only if I is the support of a positive dependence (circuit) of $\mathcal{V}$.

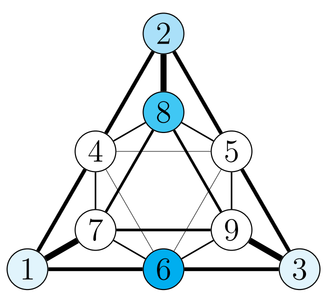
We now have the tools to connect k-graphical designs to eigenpolytopes. Recall that G has m eigenspaces, and $\boldsymbol{k} = \{2, \ldots, k\} \subset [m]$.

Theorem 3.5.3. Let $G = ([n], E, w)$ be a connected weighted graph with m eigenspaces $\Lambda_1 < \ldots < \Lambda_m$. A set $S \subset [n]$ is a (minimal) positively weighted k-graphical design of G if and only if $[n] \setminus S$ indexes the elements of $\mathcal{U}_{[m]\backslash \boldsymbol{k}}$ which lie on a face (facet) of the eigenpolytope $P_{[m]\backslash \boldsymbol{k}}$.

Proof. By definition, positively weighted k-graphical designs of G are positive dependences on the matrix $U_{\boldsymbol{k}}$. The matrices $U_{\boldsymbol{k}}$ and $U_{[m]\setminus\boldsymbol{k}}$ satisfy the hypotheses of Corollary 3.5.2: they are full rank, the first row of $U_{[m]\setminus\boldsymbol{k}}$ is the eigenvector $\mathbb{1}$, and by the orthogonality of eigenspaces, $U_{\boldsymbol{k}}U_{[m]\setminus\boldsymbol{k}}^{\top} = 0$. Therefore the faces (facets) of $P_{[m]\setminus\boldsymbol{k}}$ are dual to the dependences (circuits) of $\mathcal{U}_{\boldsymbol{k}}$ in the sense of Gale duality: S indexes the elements of $\mathcal{U}_{[m]\setminus\boldsymbol{k}}$ lying on a face (facet) of $P_{[m]\setminus\boldsymbol{k}}$ if and only if $[n] \setminus S$ indexes the support of a (minimal) dependence on $\mathcal{U}_{\boldsymbol{k}}$. □

If one allows negative quadrature weights, arbitrary graphical designs are (essentially) in bijection with the complements of hyperplanes slicing through the interior of the corresponding eigenpolytope. This broader story is briefly touched on in [6, Example 3.18] and its preceding commentary.

Example 3.5.4. We illustrate the bijection established in Theorem 3.5.3. Figure 3.8 re-exhibits the 4-graphical design, which is a circuit of $\mathcal{U}_{\{2,3,4\}}$, along with the Gale dual eigenpolytope $P_{\{1,5,6\}} \simeq P_{\{5,6\}}$. The facet which corresponds to the design is highlighted in cyan.



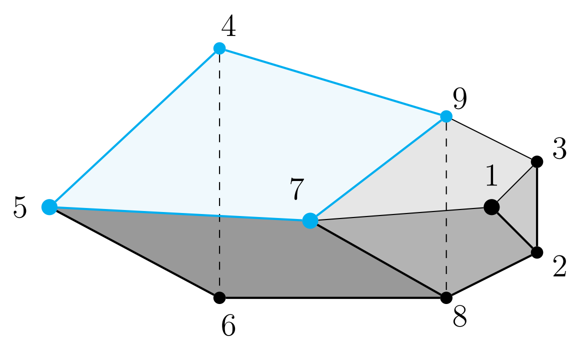


Figure 3.8: A positively weighted 4-graphical design and its corresponding facet on the Gale dual eigenpolytope. A more saturated color on a graph vertex corresponds to a larger quadrature weight.

Remark 3.5.5. The bijection established in this section remains true if $D - A$ is replaced by any symmetric operator which has $\Lambda_1 = \mathrm{span}\{\mathbb{1}\}$ as an eigenspace; for instance, the symmetric normalized adjacency matrix $D^{-1/2}AD^{-1/2}$. See [25] for more on various graph Laplacians.

Remark 3.5.6. One could also define graphical designs for positively weighted graphs using the eigenvectors of AD^{-1}, however, the framework provided by Gale duality and eigenpolytopes does not immediately apply. If the graph is not regular, the eigenspaces of AD^{-1} need not be orthogonal, hence the matrices $U_{\boldsymbol{k}}$ and $U_{[m]\setminus\boldsymbol{k}}$ need not satisfy the conditions of Theorem 3.5.1. This can be worked around with some care if one considers the dual configurations given by $U_{\boldsymbol{k}}$ and $U_{[m]\setminus\boldsymbol{k}}D^{-1}$. There are many details to this, which we do not elaborate on here.

Theorem 3.5.3 provides an upper bound to the size of a minimal k-graphical design, similar to [6, Theorem 3.14].

Theorem 3.5.7. Let $G = ([n], E, w)$ be a connected, positively weighted graph with eigenspaces $\Lambda_1 < \cdots < \Lambda_m$. For every $k \in [m-1]$ there is a positively weighted k-graphical design with at most $\sum_{i=1}^{k} \dim \Lambda_i$ vertices.

Proof. Because $\dim(P_{[m]\setminus\boldsymbol{k}}) = \sum_{i=k+1}^{m} \dim \Lambda_i$, any facet of $P_{[m]\setminus\boldsymbol{k}}$ has at least $\sum_{i=k+1}^{m} \dim \Lambda_i$ distinct vertices. By Theorem 3.5.3, any minimal positively weighted k-design then has at most $n - \sum_{i=k+1}^{n} \dim \Lambda_i = \sum_{i=1}^{k} \dim \Lambda_i$ vertices. □

We note that this bound may be tight. The example of an unweighted regular graph and an eigenspace ordering for which this bound is tight for every k given in [6, Example 3.16] is also valid here.

Example 3.5.8. We return to our running example for the last time. In the ordering specified in Example 3.4.2, Theorem 3.5.7 states that a minimal positively weighted 4-design has at most 6 vertices and is dual to a triangular facet of $P_{\{1,5,6\}}$. This eigenpolytope also has quadrilateral facets, which correspond to designs with $5 < 6$ vertices (see Figure 3.8).

We conclude this section with a few structural remarks about graphical designs that follow from the Gale duality bijection.

Remark 3.5.9. Fix an ordering $\Lambda_1 < \ldots < \Lambda_m$ of a graph $G = ([n], E, w)$. The i-th element of $\mathcal{U}_{[m]\setminus \boldsymbol{k}}$ lies in the interior of the eigenpolytope $P_{[m]\setminus \boldsymbol{k}}$ if and only if i is in the support of every k-graphical design.

We recall a quick result about combinatorial designs.

Lemma 3.5.10 (Lemma 2.4 of [6])**.** If $S \subset [n]$ is a combinatorial k-design, then so is $[n] \setminus S$.

Proof. Because $U_{\boldsymbol{k}} \perp \mathbb{1}$,

$$U_{\boldsymbol{k}} \mathbb{1}_S = 0 \iff U_{\boldsymbol{k}}(\mathbb{1} - \mathbb{1}_S) = 0 \iff U_{\boldsymbol{k}} \mathbb{1}_{[n]\setminus S} = 0$$

□

Remark 3.5.11. If $S \subset [n]$ is a combinatorial k-design, then S and $[n] \setminus S$ partition $P_{[m]\setminus \boldsymbol{k}}$ into two disjoint faces. Therefore, if G has a combinatorial k-design, no vertices lie in the interior of $P_{[m]\setminus \boldsymbol{k}}$.

We speculate that the symmetry needed for a combinatorial design to exist prevents a graph vertex from being ‘so important’ that it is in every design.

3.6 Complexity Results

The hardness of some algorithmic problems for graphical designs follows by uniting all of the established theory. We first recall some basics of polytopes; see [45] or [109] for more. We assume 0 is in the interior of every polytope. A polytope P can either be expressed as the convex hull of finitely many points, known as a $\mathcal{V}$-description, or as the bounded intersection of finitely many half-spaces, known as an $\mathcal{H}$-description. Because 0 is in the interior of $P = \operatorname{conv}(\{v_1, \ldots, v_n\})$, $P^* = \bigcap_{i=1}^n \{x : v_i^\top x \leq 1\}$ is also a polytope, known as the *dual polytope* to P. We note that $(P^*)^* = P$. A d-dimensional polytope is *simple* if every vertex is incident to exactly d edges, or equivalently, exactly d facets. We recall that a polytope is *simplicial* if each of its facets is a simplex. Simplicial polytopes and simple polytopes are dual in this sense: if $P = \text{conv}(\{v_1, \ldots v_n\})$ is simple (resp. simplicial), then $P^* = \bigcap_{i=1}^n \{x : v_i^\top x \leq 1\}$ is simplicial (resp. simple).

It was established independently in [23] and [30] that it is NP-complete to determine whether an $\mathcal{H}$-polytope is simple. The improvement to strong NP-completeness is due to [33].

Lemma 3.6.1 ([23, 30, 33])**.** The following decision problem is strongly NP-complete.

Input: A polytope P given in $\mathcal{H}$-description, where the hyperplanes are described by rational data.

Question: Is P nondegenerate (simple)?

Passing to the dual polytope provides an immediate corollary.

Corollary 3.6.2. The following decision problem is strongly NP-complete.

Input: A polytope P given in $\mathcal{V}$-description, where the vertices are rational.

Question: Is P simplicial?

We now use this corollary to show that it is strongly NP-complete to determine whether a graph has a positively weighted k-design of size smaller than the facet bound shown in Theorem 3.5.7.

Theorem 3.6.3. The following decision problem is strongly NP-complete.

Input: A connected, positively weighted graph $G = ([n], E, w)$, $w \in \mathbb{Q}^E_{>0}$ with m Laplacian eigenspaces $\Lambda_1 = \text{span}\{\mathbb{1}\} < \Lambda_2 < \ldots < \Lambda_m$, and $k \in \{2, \ldots, m-1\}$.

Question: Is there a positively weighted k-graphical design consisting of fewer than $\sum_{i=1}^k \dim(\Lambda_i)$ vertices?

Proof. We first show that this problem is in NP. Given a weight vector $a \geq 0$ with $\text{supp}(a) = S \subset [n]$, it is polynomial time in n to check whether a defines a k-graphical design by checking if $U_{\boldsymbol{k}} a = 0$ and further whether $|S| < \sum_{i=1}^k \dim(\Lambda_i)$.

To show strong NP-completeness, we will show that the decision problem in Corollary 3.6.2 is a sub-problem of the decision problem in the theorem statement. Let $P = \mathrm{conv}(\{v_1, \ldots, v_n\} \subset \mathbb{Q}^d)$ be a polytope given in $\mathcal{V}$ description with $d \leq n-2$. We note that if $d = n-1$, then the polytope P must be a simplex and hence simplicial. By Theorem 3.3.2, there is a strongly polynomial time algorithm to create a graph $G = ([n], E, w)$ with rational positive edge weights and eigenspaces $\Lambda_1 = \mathrm{span}\{\mathbb{1}\}, \Lambda_2, \Lambda_3$ for which P is affinely equivalent to $P_{\{1,3\}} \simeq P_{\{3\}}$. Consider the eigenspace ordering $\Lambda_1 < \Lambda_2 < \Lambda_3$. By Theorem 3.5.3, the facets of P are in bijection with the minimal positively weighted 2-graphical designs. A facet of P is a simplex if and only if it contains exactly d vertices. The polytope P is then simplicial if and only if every minimal positively weighted 2-graphical design has exactly $n - d = 1 + \dim(\Lambda_2)$ vertices. Thus if we could determine whether a graph $G = ([n], E, w)$ has a 2-graphical design of size smaller than the bound in Theorem 3.5.7, we could determine whether an arbitrary polytope P was simplicial. Any k-graphical design is also a k'-graphical design for all $k' < k$, so the case of general k-designs must also be hard. $\square$

We note a further straightforward consequence of Theorem 3.6.1 which we have not found explicitly stated in the literature. We also credit Alexander E. Black for making the same observation independently.

Corollary 3.6.4. The following problem is NP-hard.

Input: A polytope $P = \mathrm{conv}\{v_1, \ldots, v_n\}$ given in $\mathcal{V}$-description, where $v_i \in \mathbb{Q}^d$.

Output: A facet $F = \mathrm{conv}\{v_{i_1}, \ldots, v_{i_j}\}$ of P containing the maximum number of vertices of P among all facets.

Proof. A solution to this problem implies a solution to Corollary 3.6.2. Suppose there was an algorithm to find such a facet $F = \mathrm{conv}\{v_{i_1}, \ldots, v_{i_j}\}$. If $j > d$, then F is a non-simplex facet of P, hence P is not simplicial. If $j = d$, then every facet of P has at most d vertices by the maximality of F. Since a facet of a d-dimensional polytope must have at least d vertices, it follows that every facet is the convex hull of exactly d vertices, i.e. is a simplex. Thus P is simplicial. $\square$

Thus we can make the following translation to graphical designs.

Theorem 3.6.5. The following problem is NP-hard.

Input: A connected, positively weighted graph $G = ([n], E, w)$, $w \in \mathbb{Q}^E_{>0}$ with m Laplacian eigenspaces $\Lambda_1 = \text{span}\{\mathbb{1}\} < \Lambda_2 < \ldots < \Lambda_m$, and $k \in \{2, \ldots, m-1\}$.

Output: A minimum cardinality positively weighted k-graphical design.

Proof. The proof is nearly identical to the proof of Theorem 3.6.3, so we will be brief. A minimum cardinality positively weighted k-design is in bijection with a facet of the corresponding eigenpolytope that contains a maximum number of vertices. In strongly polynomial time, given any $\mathcal{V}$-polytope P, we can create a positively weighted graph G for which P is affinely equivalent to an eigenpolytope of G. Thus an algorithm for this problem would imply an algorithm for Corollary 3.6.4. □

Using a similar argument, we can show that it is #P-complete to count the number of positively weighted k-designs of a graph. It was shown independently in [30] and [62] that it is #P-complete to count the number of facets of a polytope given by its vertices.

Lemma 3.6.6 ([30, 62])**.** The following counting problem is #P-complete.

Input: A rational polytope P given in $\mathcal{V}$-description.

Output: Number of facets of P.

We again use Theorem 3.3.2 to hide the facet-counting polytope problem in the problem of counting graphical designs.

Theorem 3.6.7. The following counting problem is #P-complete.

Input: A connected, positively weighted graph $G = ([n], E, w)$, $w \in \mathbb{Q}^E_{>0}$ with m eigenspaces $\Lambda_1 = \text{span}\{\mathbb{1}\} < \Lambda_2 \ldots < \Lambda_m$, and an integer $k \in \{2, \ldots, m-1\}$.

Output: The number of minimal positively weighted k-graphical designs of G.

Proof. We will show that the counting problem in Lemma 3.6.6 is a sub-problem of this counting problem. Let $P = \text{conv}(\{v_1, \ldots, v_n\} \subset \mathbb{Q}^d)$ be a polytope with $d \leq n-2$. We note that if $d = n - 1$, then the polytope P must be a simplex and hence has n facets. By Theorem 3.3.2, there is a (strongly) polynomial time algorithm to create a graph $G = ([n], E, w \in \mathbb{Q}^E_{>0})$ with eigenspaces $\Lambda_1 = \operatorname{span}\{\mathbb{1}\}, \Lambda_2, \Lambda_3$ for which P is affinely equivalent to $P_{\{1,3\}} \simeq P_{\{3\}}$. Consider the eigenspace ordering $\Lambda_1 < \Lambda_2 < \Lambda_3$. By Theorem 3.5.3, the facets of P are in bijection with the minimal positively weighted 2-graphical designs. Thus any enumeration of the minimal positively weighted 2-graphical designs of G would count the facets of P, hence this counting problem must be #P-complete. This problem must be hard for any k because a k-graphical design is also a k'-graphical design for all $k' < k$. $\square$

Many algorithmic polytope questions are open when the dimension is not fixed. In particular, the complexity of listing all facets of a polytope given a vertex description is unknown, though it is widely believed to be a difficult problem. Any complexity result for the facet enumeration problem would provide a complexity result for the problem of listing all minimal k-graphical design, using the same framework as in the proofs of this section.

Remark 3.6.8. We note that it is polynomial time to find a not necessarily minimal k-graphical design. A solution to the linear program

$$\min c^\top x \qquad \text{s.t. } U_{\boldsymbol{k}} x = 0, \mathbb{1}^\top x = 1, x \geq 0 \tag{3.1}$$

provides a positively weighted k-graphical design for any cost vector $c \in \mathbb{R}^n$, though the design need not be minimum or minimal. We recall that linear programming is polynomial time by [56, 53], and moreover one can find an *extreme point solution* in polynomial time [58, Theorem 2.1.6]. The Rank Lemma from linear programming guarantees some sparsity of extreme point solutions.

Lemma 3.6.9. [58, Lemma 1.2.3] An extreme point solution x^* of

$$\min c^\top x \qquad \text{s.t. } Ax = b, x \geq 0$$

is zero on $\operatorname{corank}(A)$ coordinates.

Thus an extreme point solution of the LP in (3.1) has $n - k$ zero coordinates, which is to say the design contains k vertices. The one-norm is often used as a proxy for sparseness, but the constraints $\mathbb{1}^\top x = 1, x \geq 0$ imply that $\|x\|_1 = 1$ for all feasible x in (3.1). While it theoretically makes no sense to minimize the one-norm, doing so in practice using MATLAB and Gurobi [68, 46] has yielded very sparse graphical designs, often sparser than the guarantee of the Rank Lemma.

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