Spectral characterizations of complex unit gain graphs

Wissing, Pepijn

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Spectral Characterizations of Complex Unit Gain Graphs

PEPIJN WISSING

TILBURG UNIVERSITY

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PEPIJN WISSING

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PROMOTOR: prof. dr. ir. Edwin van Dam

COPROMOTOR: dr. ir. ing. René Peeters

PROMOTIECOMMISSIE: prof. dr. Etienne de Klerk
prof. dr. ir. Willem Haemers
prof. dr. ir. Jack Koolen
dr. Krystal Guo
dr. ir. Pieter Kleer

Spectral Characterizations of Complex Unit Gain Graphs

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Pepijn Wissing
Cesena, August 2022

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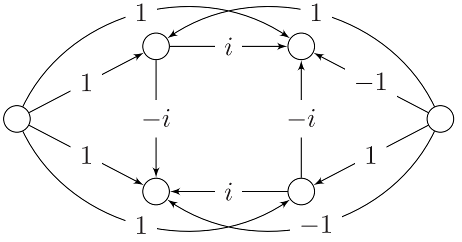
CHAPTER 1

Introduction

Graphs are, at their essence, structures containing sets of objects in which some pairs of the objects are in some sense related. The objects are commonly abstracted and called *vertices*, and each of the related pairs of vertices is called an *edge*. Built on this foundation are a frankly alarming number of subtly distinct subclasses and properties, including the class that acts as the backbone of this thesis: *gain graphs*.

Informally, a gain graph is obtained by assigning a direction and a weight (a complex number with unit length) to every edge that is present in a given graph. They are usually represented either diagrammatically, such as in Figure 1.1, or by some matrix, say A. Since the latter is square, one may compute its *eigenvalues* λ, that satisfy $Av = \lambda v$ for some *eigenvector* v. Of primary concern to this thesis is the structural information that may be extracted from a gain graph's collection of eigenvalues, with the ultimate goal of finding gain graphs whose eigenvalues contain sufficiently much information that one may uniquely reconstruct said gain graph when given only its eigenvalues.



$$A(\Psi) = \begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & -i & -1 & 0 & i \\ 1 & i & 0 & 1 & -i & 0 \\ 0 & -1 & 1 & 0 & -1 & 1 \\ 1 & 0 & i & -1 & 0 & -i \\ 1 & -i & 0 & 1 & i & 0 \end{bmatrix}$$

Figure 1.1 – A gain graph Ψ and its gain matrix $A(\Psi)$

1.1 Basic definitions

Let us first thoroughly discuss the terminology and notation. Most of the concepts below are well-known and will not always be explicitly referenced. For more detail, the reader is referred to e.g., Bondy and Murty [9] or any other recent book on graph theory.

1.1.1 Graph definitions

A *graph* of order n is denoted $G = (V, E)$, where V (sometimes specified as $V(G)$) is the *vertex set*, typically denoted $V = \{1, \ldots, n\}$. $E \subseteq \binom{V}{2}$ is called the *edge set* of G. Similarly to $V(G)$, we will sometimes specify the associated graph G as $E(G)$. In the case of an undirected graph G, $E(G)$ consists of unordered pairs of vertices, usually denoted (u, v) for $u, v \in V$. For clearness, we will only use the word "graph" when it concerns an undirected graph.

A *directed graph* or *digraph* of order n is denoted[1] $D = (V, E)$. However, in the directed case, $E \subset V \times V$ consists of ordered pairs uv of vertices, called *arcs* or *directed edges*. Here, u is called the *initial vertex* and v is called the *terminal vertex* of uv. If both $uv \in E$ and $vu \in E$, we say that (u, v) is a *digon* in D.

A *sign function* $\sigma : E(D) \mapsto \{\pm 1\}$ assigns a (positive or negative) sign to every edge in a digraph. The pair $\Phi = (D, \sigma)$ is said to be a *signed digraph.* A large portion of this thesis will use a Hermitian representation of such signed digraphs, that corresponds naturally to a gain graph (see below) whose gain values are restricted to $\mathbb{T}_6 = \{\exp(i\pi k/3) \mid k = 1, \ldots, 6\}$.

In general, such a *complex unit gain graph* is said to be the pair $\Psi = (G, \psi)$, where G is a bidirected graph and $\psi : E(G) \to \mathbb{T} = \{z \in \mathbb{C} \ : \ |z| = 1\}$ is a *gain function* with the property that $\psi(uv) = \psi^{-1}((v, u))$. Here, a *bidirected* graph is a directed graph such that $uv \in E$ if and only if $(v, u) \in E$.

We may sometimes be interested in the *underlying graph* of D, Φ or Ψ. Let $\Gamma(\cdot)$ be the operator that transforms a digraph into its underlying graph. That is, given D, the graph $G = \Gamma(D)$ is obtained by including $\{u, v\}$ in $E(G)$ for every $uv \in E(D)$ and discarding any duplicate edges. With slight abuse of notation, $\Gamma(\Phi) = \Gamma(D)$ if $\Phi = (D, \sigma)$ and similarly $\Gamma(\Psi) = \Gamma(G)$. To circumvent some of the more

[1] Some of the cited literature considers *mixed graphs*, which are defined to be an ordered triple (V, E, A), where V is the vertex set, E is the undirected edge set and A is the directed edge set. Since a single bidirected edge is, for our purposes throughout this thesis, equivalent to two arcs whose directions are reversed, we consider the class of mixed graphs equivalent to the class of digraphs.

tedious technicalities, we will sometimes use the word *edge* to indicate an edge in the underlying graph, when the context is clear. Finally, a *loop* is an edge of which the terminal vertex equals the initial vertex. Throughout, we will not allow graph, digraph or gain graph to contain loops.

1.1.2 Graph theoretical properties

A given graph G is said to be *k-regular* if every vertex has k neighbors and *bipartite* if it contains no odd-sized cycles. Gain graphs are said to be k-regular and bipartite when their underlying graphs are. Finally, a (signed) digraph is said to be *oriented* when it contains no digons.

If $D = (V, E)$ and let $W \subset V$, then we denote the *(vertex-)induced subgraph* that is obtained by removing any vertices in $V \setminus W$ and removing any edges that are incident to a vertex in $V \setminus W$ as $D[W]$. The notation carries over to (gain) graphs in the obvious way. A *subgraph* (notably: not induced) is obtained by additionally removing digons or arcs without removing either of the incident vertices, and will almost exclusively come up in the context of elementary subgraphs (see Section 1.1.4). The *symmetric subgraph* $G(D)$ of a digraph D is obtained by retaining only the digons in $E(D)$.

Two digraphs D and D' are said to be *isomorphic* if there exists a bijection $f : V(D) \to V(D')$ such that $uv \in E(D)$ if and only if $f(u)f(v) \in E(D')$. For a pair of signed digraphs Φ and Φ', it is additionally required that $\sigma(uv) = \sigma(f(u)f(v))$ for all $uv \in E(\Phi)$; for a pair of gain graphs Ψ and Ψ', it is similarly required that $\psi(uv) = \psi(f(u)f(v))$ for all $uv \in E(\Psi)$ In case the graph/digraph/gain graph is mapped onto itself, f is called an *automorphism*. A graph is said to be *symmetric* if it has a non-trivial automorphism.

The *converse* of a (signed) digraph D is denoted D^c, and is obtained by reversing the direction of all arcs. A (signed) digraph that is isomorphic to its converse is said to be *self-converse*.

1.1.3 Eigenvalues

A *eigenvalues* λ of a square matrix A satisfy $Av = \lambda v$, for some *eigenvector* v. They may be obtained as the roots of the *characteristic polynomial*

$$\chi(\lambda) = \det(\lambda I - A) = \lambda^n + a_1\lambda^{n-1} + \ldots + a_n. \tag{1.1}$$

The collection of eigenvalues is also called the *spectrum*, often denoted

$$\Sigma = \left\{\theta_1^{[m_1]}, \ldots, \theta_k^{[m_k]}\right\},$$

where $\theta_1 > \ldots > \theta_k$ are the k distinct eigenvalues, whose multiplicities are $m_1, \ldots, m_k$.

The spectrum of (signed) digraph or gain graph is said to be the spectrum of the associated matrix (the Hermitian adjacency matrix H, Eisenstein matrix $\mathcal{E}$ or gain matrix A; formal definitions appear later in this chapter). The matrices associated with the various kinds of graphs are all[2] Hermitian, and thus diagonalizable [11] with real eigenvalues.

A useful property of Hermitian matrices is known as *eigenvalue interlacing* (originally due to Cauchy and concisely surveyed by Haemers [55]).

Lemma 1.1. *[55, 43] Suppose A is a Hermitian $n \times n$ matrix with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$. Then the eigenvalues $\mu_1 \geq \ldots \geq \mu_m$ of a principal submatrix of size m satisfy $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$ for $i \in [m]$.*

This property is extremely useful when it comes to forbidden subgraph proofs, and will be used extensively in Chapters 2, 4 and 7.

Two (signed) digraphs or two gain graphs are said to be *cospectral* when their spectra (or, equivalently, characteristic polynomials) are equal. That is, Ψ and Ψ' are cospectral when λ occurs as an eigenvalue of Ψ with multiplicity m if and only if it occurs as an eigenvalue of Ψ' with multiplicity m, for all eigenvalues λ. Note that similar matrices are cospectral, and that the switching operations in Definitions 1.5 and 1.6 are essentially similarity transformations.

As is convention, $\rho(D)$ denotes the spectral radius of D, i.e., its largest eigenvalue in absolute value, and the spectrum is said to be *symmetric* if it is invariant under multiplication by -1.

1.1.4 Cycles and gains of walks

Of essential interest, from a spectral point of view, is the gain of a cycle in G. Let C be a subgraph of G that is a cycle and let $C^{\rightarrow}$ denote a directed cycle obtained from C by orienting all edges of C in the same direction. That is, every vertex in $C^{\rightarrow}$ has

[2] With the exception of Section 1.3, which serves as an introductory example.

indegree and outdegree equal to 1. Then the gain of $C^{\rightarrow}$ is defined as

$$\phi(C^{\rightarrow}) = \prod_{e \in E(C^{\rightarrow})} \psi(e).$$

In case C is traversed in the reverse direction, say by $C^{\leftarrow}$, then $\phi(C^{\leftarrow}) = \overline{\phi(C^{\rightarrow})}$. Since the traversal direction does not affect the (primarily interesting, see Theorem 1.2) real part of the cycle gain, the direction is usually omitted.

Whenever two cycles C_1 and C_2 intersect on a path of length at least 2, their symmetric difference $C_1 \ominus C_2$ is, again, a cycle. In this way, the collection $\mathcal{C}$ of all cycles in a graph (also called the *cycle space*) may be written as the symmetric differences of cycles in the *cycle basis* $\mathcal{B} \subseteq \mathcal{C}$. Specifically, $\mathcal{B}$ is a smallest set of cycles that generates the cycle space. Moreover, one may compute the gain of the new cycle by taking the product of the gains of the old cycles, making sure that their intersection is traversed in opposite directions. Loosely put, we have $\phi(C_1 \ominus C_2) = \phi(C_1^{\rightarrow})\phi(C_2^{\leftarrow})$.

Crucially, the gains of cycles are closely related to the spectrum of a gain graph, via the well-known Harary-Sachs coefficients theorem. A graph H is called an elementary graph if each of its connected components is either an edge or a cycle. The characteristic polynomial of a gain graph may be obtained from its elementary subgraphs as follows.

Theorem 1.2. *[91] Let Ψ be a unit gain graph with underlying graph G and characteristic polynomial $\chi(\lambda)$ as in* (1.1)*. Then*

$$a_j = \sum_{H \in \mathcal{H}_j(G)} (-1)^{p(H)} 2^{c(H)} \prod_{C \in \mathcal{C}(H)} Re\left(\phi(C)\right), \tag{1.2}$$

where $\mathcal{H}_j(G)$ is the set of all elementary subgraphs of G with j vertices, $\mathcal{C}(H)$ denote the collection of all cycles in H, and $p(H)$ and $c(H)$ are the number of components and the number of cycles in H, respectively.

Note that for the case of signed digraphs, the above may be slightly rewritten.

Theorem 1.3. *Let Φ be a signed digraph with underlying graph G. Let $\chi(\lambda) = \lambda^n + a_1\lambda^{n-1} + \ldots + a_n$ be the characteristic polynomial of Φ. Then the coefficients a_j may be calculated as*

$$a_j = \sum_{H \in \mathcal{H}_j(G)} (-1)^{p(H)+n(H)} 2^{c(H)-z(H)}, \tag{1.3}$$

(a) 3-pan (b) Gem

Figure 1.2 – Two small graphs and their names.

Gain	Drawing	Type (SDG)
$\psi(uv) = 1$	u ——— v	Positive digon
$\psi(uv) = -1$	u - - - - - - v	Negative digon
$\psi(uv) = \omega$	$u \longrightarrow v$	Positive arc
$\psi(uv) = -\omega = \varphi^2$	$u \dashrightarrow v$	Negative arc
$\psi(uv) = \gamma$	$u \cdots\cdots\!\rightarrow v$	-
$\psi(uv) = 1$, fixed ex ante	u **━━━** v	-

Table 1.1 – Drawing conventions. The type concerns Chapter 4.

where $n(H)$ and $z(H)$ respectively denote the number of negative cycles and non-real cycles in $\mathcal{C}_H$.

1.1.5 Conventions

Throughout, the identity matrix, the all-ones matrix and the zero matrix are denoted I, J and O, respectively. Occasionally, a subscript is added to clarify its dimensions. We often denote by respectively $\varphi = \exp(2i\pi/3), \omega = \exp(i\pi/3)$ and $\gamma = \exp(i\pi/4)$ the third, sixth and eighth roots of unity.

Finally, we include a few often-used graphs and their names. A complete graph of order n is denoted K_n, and a complete k-partite graph is denoted $K_{n_1,\dots,n_k}$. Further, the empty graph is denoted O_n, the path is denoted P_n, and a cycle is denoted C_n. The *transitive tournament* T_n is the digraph whose arc set is exactly $E(T_n) = \{uv \mid u \leq v \text{ for } u, v \in [n]\}$. The remaining two named graphs are shown in Figure 1.2.

We conclude by offering an overview of the drawing conventions used in illustrations throughout, shown in Table 1.1.

1.2 Spectra of graphs

For decades, generations of mathematicians have investigated the interplay between the eigenvalues of a graph and its structural characteristics. Accordingly, this connection is used in several computationally intensive fields such as combinatorial optimization. Paraphrasing Mohar and Poljak [85], one of the key applications is the possibility of the change to a "continuous optimization," of which a classical example is Lovász ϑ-function [77]. Its use as a bound gives rise to polynomial time algorithms for determining the stability number, or the chromatic number in perfect graphs. Similar approaches appear in relation to bipartion width, max-cut, and partition, among others. [11]. Moreover, eigenvalues of graphs are also related to various design-oriented disciplines like coding theory [102].

Indeed, the eigenvalues of a graph carry valuable information. This includes various classical results, like the observation that a graph is bipartite if and only if its spectrum is symmetric (see Chapter 6). Now, it would be natural to ask whether or not some graphs may have collections of eigenvalues (also called the *spectrum*) that contain enough information, in terms of structural properties that may be derived from them, that they are effectively the only graphs with those spectra. In other words, graphs that are *characterized* or *determined* by their spectrum.

The question was, to our knowledge, first asked in 1956, when Günthard and Primas [49] raised the issue in a paper that relates the theory of graph spectra to Hückel's rule [67] in chemisty. Another occurrence of this question from that time in physics has to do with the question whether one can hear the shape of a drum. Fisher [38] modeled a drum as a graph, and showed that the sound the drum makes is characterized by the eigenvalues of this graph. For about a year, it was believed that no two graphs would share a spectrum. Examples to the contrary would pop up sporadically, the smallest one being the so-called "Saltire pair" in Figure 1.3. Later, Schwenk [97] concluded that "almost all trees have a *cospectral mate*".

Over the years, this has developed into a considerable body of research. However, there is still no consensus as to statements for general graphs, analogous to Schwenk's result. The fraction of graphs that is known to be determined by its spectrum (hereafter: DS) goes to zero as their order goes to infinity, but so does the fraction of graphs that have known cospectral mates. Thus, are almost all graphs DS, are almost no graphs DS, or is neither true? It has been conjectured [27, 28], that the fraction of DS graphs goes to one, although this has remained an open problem.

Figure 1.3 – A pair of graphs which have the same spectrum.

1.3 Directed graphs: a warm-up exercise

Far less is known about spectral characterizations of directed (or mixed) graphs. Part of the problem is that it is as yet unclear which matrix best reflects the characteristics of a directed graph in its eigenvalues. Consider, for example, the usual adjacency matrix.

Definition 1.1. *Let $D = (V, E)$ be a digraph of order n. Then its $n \times n$ adjacency matrix $A(D)$ is defined by*

$$[A]_{uv} = \begin{cases} 1 & \text{if } (u,v) \in E \\ 0 & \text{otherwise.} \end{cases}$$

Since, with respect to digraphs, $(u, v) \in E$ does not necessarily imply $(v, u) \in E$, A is in general not symmetric. As a consequence, its eigenvalues are not necessarily real and many of the usual tools (such as eigenvalue interlacing and the typical counting of order-k closed walks by $\operatorname{tr}\left(A^k\right)$) are lost.

In general, directed graphs that are determined by their adjacency spectrum appear[3] to be few and far between. What is worse, claims have turned out to be considerably harder to formalize for directed graphs of arbitrary order. Even for extremely narrow families, one needs reasonably big guns to even make a dent. We illustrate this point by proving that the directed cycle $\overrightarrow{C}_n$ is determined by its adjacency spectrum, as a warming-up exercise. The eigenvalues λ_j of $\overrightarrow{C}_n$ are given by [72]

$$\lambda_j = \cos\left(2\pi \frac{j}{n}\right) + i \ \sin\left(2\pi \frac{j}{n}\right), \text{ for } j \in [n]. \tag{1.4}$$

[3]Although the performed enumeration studies (see, e.g., [52]) have been limited to digraphs of small order, this conclusion seems likely as the fraction of digraphs with unique characteristic polynomials (w.r.t. $A(D)$) goes to zero at a rapid pace.

While eigenvalue interlacing does not generally apply to the adjacency matrices of directed graphs, one may use their spectral radii $\rho(\cdot)$ to work along a familiar line. In particular, the following consequence of the well-known Perron-Frobenius theorem is used.

Lemma 1.4. *Let D be a directed graph and let D' be obtained from D by removing at least one arc. Then $\rho(D') < \rho(D)$.*

The following conclusion now follows easily by observing that 1 is effectively the smallest possible spectral radius of any strongly connected component.

Proposition 1.5. *Let D be a digraph of order n. If D is strongly connected and D has spectral radius 1, then $D = \overrightarrow{C_n}$.*

Proof. Assume that D is strongly connected, and suppose that $D \neq \overrightarrow{C_n}$. Then there exists an integer k with $2 \leq k \leq n$ such that $\overrightarrow{C_k}$ can be obtained by removing one or more arcs and $n-k$ vertices from D. Indeed, note that otherwise at least one vertex has outdegree zero and thus D would not be strongly connected. By Lemma 1.4, if D' is obtained from D by deleting one or more edges or nodes, then $\rho(D') < \rho(D)$. Finally, since $\rho(\overrightarrow{C_k}) = 1$ for any $k > 1$, it follows that $\rho(D) > 1$, contradiction. □

Now, one may consider the order of strongly connected components in a digraph to conclude that the directed cycle of arbitrary order has a uniquely occurring spectrum.

Proposition 1.6. *$\overrightarrow{C}_n$ is determined by its adjacency spectrum.*

Proof. Let D be cospectral to $\overrightarrow{C}_n$. As a strongly connected digraph has an irreducible adjacency matrix, it follows by the Perron-Frobenius theorem that any strongly connected component has a real, positive spectral radius. Since only $\lambda_1 = 1$ is strictly real and positive, it follows that D contains exactly one strongly connected component. Moreover, since none of the λ_j are zero, D contains no components that are not strongly connected. The desired conclusion now follows by Proposition 1.5. □

While the above proves spectral characterization w.r.t. the adjacency matrix, it mostly abuses a few characteristics that are specific to the directed cycle, and has proven difficult to extend to broader families of digraphs. As such, we explore the possible benefits of the Hermitian adjacency matrix.

1.4 The Hermitian adjacency matrix

A promising candidate to work around some of the shortcomings of the adjacency matrix is the Hermitian adjacency matrix (usually simply *the Hermitian* for short), introduced independently by Guo and Mohar [51] and Liu and Li [76].

Definition 1.2. *[51, 76] Let $D = (V, E)$ be a digraph of order n. Define the Hermitian $H = H(D)$ as the $n \times n$ matrix with entries*

$$[H]_{uv} = \begin{cases} 1 & \textit{if } (u,v) \in E \textit{ and } (v,u) \in E, \\ i & \textit{if } (u,v) \in E \textit{ and } (v,u) \notin E, \\ -i & \textit{if } (u,v) \notin E \textit{ and } (v,u) \in E, \\ 0 & \textit{otherwise.} \end{cases} \tag{1.5}$$

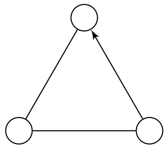
Conceptually, the premise is fairly simple: by encoding into the adjacency matrix not just whether a given vertex is reachable from another, but also whether or not the reverse direction might be traveled as well, a digraph is described unambiguously by this matrix. Moreover, since H is, by definition, equal to its conjugate transpose H^*, the matrix is Hermitian and therefore has certain algebraic benefits over the traditional adjacency matrix, such as being diagonalizable with real eigenvalues [11].

From a spectral analysis point of view, there are some drawbacks to the departure from real matrices. Out of the classical results, probably the most notable absentee would be the Perron-Frobenius theorem, though many of the spectral results that experienced graph theorists might be used to do not necessarily carry over either. For example, while it is well known that the A-spectrum of a graph is symmetric around the origin if and only if the graph is bipartite, this implication only goes one way with respect to H.

Lemma 1.7. *Let D be a bipartite digraph. Then its H-spectrum is symmetric. That is, λ is an eigenvalue of $H(D)$ with multiplicity m if and only if $-\lambda$ is also an eigenvalue of $H(D)$ with multiplicity m.*

Lemma 1.8. *Let D be an oriented digraph, i.e., $(u, v) \in E \implies (v, u) \notin E$. Then its H-spectrum is symmetric.*

However, neither of the reverse implications holds, as is evident by considering the digraph in Figure 1.4. For our purposes, one of the foremost perks of using a Hermitian matrix is that eigenvalue interlacing is applicable [52, 51].



$$H(D) = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & -i \\ 1 & i & 0 \end{bmatrix}$$

Figure 1.4 – A digraph D whose H-spectrum is $\{-\sqrt{3}, 0, \sqrt{3}\}$

1.5 Signed directed graphs

By equipping an undirected graph with a sign function $\sigma : E \mapsto \{\pm 1\}$, Zaslavsky [109] introduced the concept of *signed graphs*; an idea that is actively being researched to this day [6]. While this notion is easily incorporated in the directed graph paradigm, the Hermitian H does not lend itself well to the natural inclusion of said signs into the defining matrices of *signed directed graphs.* Indeed, note how 'simply' multiplying the entries of the negative arcs with -1, as is customary in the adjacency matrices of signed graphs, would, in terms of the Hermitian adjacency matrix, reverse the direction of the arc, rather than actually signifying the desired sign.

However, since the task of encoding an arc could effectively be performed by any complex number, one quickly arrives at an intuitive candidate. Indeed, note that a vertex can be the initial vertex of a positive arc, the terminal vertex of a positive arc, incident to a positive arc, and all of their respective negative counterparts. As there are six vertex-edge incidence relations, it would make sense to encode these relations by the sixths roots of unity, also known as the unit Eisenstein integers [45]. This translates to the usual element wise product to the 'new' Hermitian adjacency matrix N [84].

Definition 1.3. *Let $D = (V, E)$ be a digraph of order n with sign function $\sigma : E \mapsto \{\pm 1\}$, and let $\Phi = (D, \sigma)$ be a signed directed graph. Let $\omega = \exp(i\pi/3)$ and define the Eisenstein matrix $\mathcal{E} := \mathcal{E}(\Phi)$ as the $n \times n$ matrix with entries*

$$[\mathcal{E}]_{uv} = \sigma(u,v) N_{uv}, \;\; \textit{where } [N]_{uv} = \begin{cases} 1 & \textit{if } (u,v) \in E \textit{ and } (v,u) \in E, \\ \omega & \textit{if } (u,v) \in E \textit{ and } (v,u) \notin E, \\ \bar{\omega} & \textit{if } (u,v) \notin E \textit{ and } (v,u) \in E, \\ 0 & \textit{otherwise.} \end{cases} \tag{1.6}$$

An interesting feature of $\mathcal{E}$, compared to H and N, is that the set of allowed entries is multiplicative. That is, the nonzero entries of $\mathcal{E}$ are all members of $\mathbb{T}_6 :=$

$\{\exp(i\pi k/3) \ : \ k = 1, \ldots, 6\}$. One of the practical consequences of this property is that one may without loss of generality assume that an arbitrary spanning tree consists of only positive edges (or, in fact, any desired edge type.) On the flip side, the possibility for admissible switches (see Section 1.7) opens up tremendously, which is especially undesirable for those interested in the classical notion of spectral characterization.

1.6 Complex unit gain graphs

In hindsight, all of the objects discussed so far have been special cases of so-called *complex unit gain graphs* [110, 91]. Let G be a bidirected[4] graph, and let $\psi : E \to \mathbb{T} = \{z \in \mathbb{C} \ : \ |z| = 1\}$ be a *gain function*, with the property that the product of the gain $\psi(u, v)$ of an arc (u, v) and its converse arc (v, u) equals 1. That is, $\psi(v, u) = \psi(u, v)^{-1}$ for all $(u, v) \in E$. Then the pair $\Psi := (G, \psi)$ is known as a complex unit gain graph (usually simply "gain graph"). By design, the corresponding *gain matrix*, whose u, v entry is simply set to $\psi(u, v)$, is Hermitian, and the discussion above applies.

Originally due to Zaslavsky [110], *biased graphs* have been around for some time. Much of the theory of gain graphs is effectively a special case of that of biased graphs; the latter being defined as a graph with a designated linear subclass of *balanced* cycles[5], where the balanced cycles of the former happen to be a linear class. The spectral properties of gain graphs have been an active field of research ever since the initial article to that goal by [91]. Some interesting recent advances include [7, 68, 78].

While various links between graph theory and (finite) geometry have been known for a long time, gain graphs offer an interesting new such link. Specifically, there are two kinds of matroids associated with a gain graph [111], the so-called *frame matroid* and *lift matroid*, that relate to (real) systems of hyperplanes [112] of the form $x_i = \psi(i, j)x_j$ and $x_i = x_j + \psi(i, j)$, respectively. This thesis does not engage with said matroids, but we do find another interesting parallel between gain graphs with particular spectra and systems of lines in complex space.

Note that indeed, the Hermitian adjacency matrix H and the Eisenstein matrix $\mathcal{E}$ are effectively special cases of a complex unit gain graph. In retrospect, one may think of these objects as if they were 'restricted' gain graphs, whose edge gains belong to a subset of $\mathbb{T}$. While the nonzero entries of Ψ and $\mathcal{E}$ belong to abelian groups, the entries

[4]Bidirected in the sense that an arc (u, v) occurs if and only if (v, u) does, as well.

[5]A cycle is said to be *balanced* if the product of its edge gains in a consistent direction equals 1.

Figure 1.5 – Two isomorphic graphs

of H do not; this is the origin of the main distinction between the three otherwise highly similar concepts, in terms of spectral determination.

1.7 Spectral determination and switching

From the outset, one of the intended goals of this thesis has been classification of graphs that are determined by their spectra; whose spectra occur *uniquely.* One of the first obstacles that one faces, in this regard, is related to the representation of graphs by matrices. All of the graphs treated in this thesis are effectively *unlabeled*, i.e., any vertex only differs from another in its relations to their mutual complement. However, in order to obtain the usual matrix representation, one must effectively assign a label to each vertex. And while the distribution of labels is of no consequence to the obtained spectrum, the corresponding matter of identification is non-trivial.

Indeed, while one would like to say *"spectrum X corresponds to that matrix Y and thus to graph G,"* it is almost always the case that spectrum X may belong to distinct matrices $Y_1, Y_2, Y_3, \ldots, Y_M$, each of which represents the graph G. If this happens, the rows and columns of Y_2 may be relabeled such that $Y_2 = Y_1$. This is known as *isomorphism* and is shown in Figure 1.5; a formal definition appeared in Section 1.1. As such, the following definition of a graph that is determined by its spectrum is customarily used.

Definition 1.4. *A graph G is said to be determined by its spectrum when it is cospectral to a graph G' if and only if G is isomorphic to G'.*

Effectively, it boils down to a question of equivalence. Indeed, if two matrices are 'close enough' to one another that their rows and columns may be permuted to make them coincide on all entries, they are equivalent in the sense that they represent the same graph, and thus are considered 'the same' for the sake of spectral characterization.

Upon entering the realm of (restricted) gain graphs, one has more of these questions to consider. In particular, taking the transpose of any matrix trivially does not affect the spectrum, while this operation generally does mutate (for example) the digraph the matrix represents. Moreover, for most gain graphs and Hermitian representations of (signed) digraphs, a phenomenon known as *gain switching* often yields a plethora of distinct, yet very closely related graphs that are somewhat trivially cospectral mates; so-called *switching equivalent* graphs. Similarly to the various kinds of switching in traditional graph theory, such as Godsil-McKay switching [44] or Seidel switching [75], the current version almost always changes the digraph, but never changes its eigenvalues. While 'traditional' switching removes some edges and adds others, *gain-switching*, as the operation was originally named by Zaslavsky [110], exclusively changes the gain of an edge and, consequently, the type or direction of the corresponding edge/arc in the (signed) digraph that might be represented by it.

In terms of the Hermitian adjacency matrix, this amounts to the following.

Definition 1.5. *[51] A four-way switching is the operation of changing a digraph D into the digraph D' by choosing an appropriate diagonal matrix S with $S_{jj} \in \{\pm 1, \pm i\}$, $j = 1, \ldots, |V(D)|$, and setting $H(D') = S^{-1}H(D)S$, and possibly taking the transpose. Informally, S is appropriate when $H(D')$ is a Hermitian adjacency matrix.*

Two digraphs are now said to be *switching equivalent* if they can be obtained from one-another via a series of four-way switches. Note that indeed, the spectrum will clearly be left unchanged, since the above are effectively a series of similarity transformations and possibly a transposition.

Example 1.1. *Consider the two digraphs in Figure 1.6. Their respective Hermitian*

(a) **(b)**

Figure 1.6 – Two switching equivalent digraphs.

adjacency matrices satisfy the equation

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -i \end{bmatrix}^{-1} \begin{bmatrix} 0 & 1 & i \\ 1 & 0 & i \\ -i & -i & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -i \end{bmatrix} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}, \tag{1.7}$$

which means that (b) is obtained from (a) by a four-way switching.

Note that not any diagonal matrix $S \in \{\pm 1, \pm i\}^{n \times n}$ is necessarily appropriate. If, for example, $S_{uu} = 1$, $H(D)_{uv} = i$ and $S_{vv} = i$, then $H(D')_{uv} = 1 \cdot i \cdot i = -1$, and thus $H(D')$ would not be the Hermitian adjacency matrix of a digraph. In rather exceptional cases, this leads to such Hermitian adjacency matrices that do not admit any (non-identity) switching; this phenomenon is exploited in Chapter 2.

However, whereas the set of nonzero entries of H is not multiplicative, thus allowing for the above exception, both $\mathcal{E}$ and ψ are defined on multiplicative groups. While the former is finite and the latter is not, their respective switching operations are effectively the same. Originally due to Zaslavsky [110], *gain switching* may be defined as follows.

Definition 1.6. *Let Ψ be a gain graph, and let Z be a diagonal matrix with $Z_{jj} \in \mathbb{T}$ for $j = 1, \ldots, |V(\Psi)|$. Gain switching is said to be the operation that changes Ψ into Ψ' by setting $A(\Psi') = Z^{-1}A(\Psi)Z$, and possibly taking the transpose. Note that if $\psi(u,v) \in \mathbb{T}_6$ for every $u, v \in V$ and $Z_{jj} \in \mathbb{T}_6$ for every j, then both Ψ and Ψ' are signed digraphs.*

Formally, we then have:

Definition 1.7. *Two gain graphs are said to be switching isomorphic if one may be obtained from the other by a sequence of diagonal switches, possibly followed by relabeling the vertices. Switching isomorphism of Ψ and Ψ' is denoted $\Psi \sim \Psi'$.*

Since switching equivalence is transitive, one may keep switching along different cuts to obtain yet more switching equivalent gain graphs. Since the values of Z do not need to be further constrained in order for Ψ' to be a gain graph (resp. signed digraph), it follows that for any non-empty gain graph (resp. signed digraph), one can find a partner to which it is switching equivalent, but not isomorphic. This is discussed in detail in Section 4.5.1. Thus, one's definition of spectral determination[6] should be amended.

[6] A H-parallel to Definition 1.8 is referred to as 'weakly determined by its H-spectrum' in Chapter 2 and appeared in [83].

Definition 1.8. *A gain graph Ψ is said to be determined by its spectrum if it is switching isomorphic to every gain graph Ψ' to which it is cospectral. Similarly, if Ψ and all Ψ' are signed digraphs, then it is said to be Determined by the Eisenstein Spectrum (DES).*

While clearly weaker than Definition 1.4, it is similar in spirit. That is, gain graphs (resp. signed digraphs) that are effectively equal up to a similarity transformation are considered to be 'the same,' for the purposes of spectral characterization.

1.8 Contributions and Overview

We provide a concise overview of the main contributions of each chapter.

While the later parts of this thesis consider spectral characterizations up to switching equivalence, Chapter 2 is concerned with the conception of an infinite family of connected digraphs whose Hermitian spectra occur uniquely up to isomorphism. That is, a family that is *strongly determined by its H-spectrum.* Such a family is obtained by effectively taking lexicographic products of a key digraph, which is named the *negative tetrahedron,* with a selection of empty graphs. This operation is referred to as *twin expansion.*

As an intermediate result, we determine all digraphs whose H-spectra have precisely one negative eigenvalue. If twin vertices are not allowed, this collection contains exactly four members, which are all of order at most 4. Exactly one of them has rank 4: the negative tetrahedron. Since twin expansion does not affect the rank, nor the number of positive (eq. negative) eigenvalues, it then follows that the only digraphs whose H spectrum contains exactly one negative and three positive eigenvalues are those that are twin expansions of the negative tetrahedron. To conclude the chapter, we determine which of these expansions may be cospectral to one another and which, conversely, have unique spectra.

It is easy to see that a digraph (or, equivalently, a mixed graph) is strongly determined by its H-spectrum only if it is isomorphic to its converse, in which case it is said to be *self-converse.* Thus, an interesting question that comes up in the discussion of Chapter 2 is: *how rare are self-converse digraphs?* Chapter 3 considers the details of this question and provides an elegant proof to show that it is a rare property, in the sense that the fraction of digraphs that satisfies it goes to zero when the order increases.

In Chapter 4, we shift our focus to signed digraphs and their Eisenstein matrices. We first provide a classification of signed directed graphs that satisfy particular spectral conditions. By fixing, without loss of generality, the gains of a spanning tree and applying eigenvalue interlacing, we classify all signed directed graphs whose rank is 2 or 3. The characterization of all such signed digraphs is rather concise, and may be described as twin expansions of either an edge, a triangle, or the transitive tournament of order four. Subsequently, we provide an extensive discussion of clique expansions of the 5-cycle and the 4-path to characterize the minimally dense signed directed graphs that have exactly 1 or 2 non-negative $\mathcal{E}$-eigenvalues.

The above properties are then used to consider signed digraphs with spectra that occur uniquely, up to switching equivalence. Through a series of counterexamples, we show that the discussed low rank signed digraphs are not, in general, determined by their spectra. However, by applying a sequence of counting arguments to the lists obtained above, we are then able to prove that, among others, several of the families with 2 non-negative eigenvalues are determined by their spectrum. Specifically, in addition to a number of sporadic examples, we find several arbitrarily large graphs, obtained as clique expansions of C_4, P_4 or C_5, that admit signed digraphs cospectral only to switching equivalent signed digraphs.

For the final three chapters of the thesis, we investigate complex unit gain graphs in their least restricted form. That is, the group of admissible gains now contains all complex numbers of unit norm. As a consequence of the shift to weights with a continuous nature, the usual exhaustive search methods - that one so often entertains in the initial search for a foothold - no longer work. Chapter 5 paints the broad strokes of an application of the well-known optimization procedure known as *simulated annealing* that may be applied to search for gain graphs with given properties.

Subsequently, in Chapter 6, we consider three forms of symmetry that are applicable to general gain graphs, namely structural symmetry, spectral symmetry and sign-symmetry; in particular, we study the relationships between them. We show that a graph G is underlying only to spectrally symmetric gain graphs if and only if it is bipartite, and that every graph is underlying to some spectrally symmetric gain graphs. Then, we consider a number of doubling operations whose origin lies with the recursive construction of Hadamard matrices. By design, these constructions yield gain graphs with symmetric spectra. While most of them also implicitly yield sign-symmetric gain graphs, we prove that a subtle adaptation of Sylvester's double transforms an arbitrary gain graph into infinitely many switching-distinct gain graphs that are not sign-symmetric.

Finally, in Chapter 7, we venture to classify various families of unit gain graphs, with two distinct eigenvalues; a property that really only occurs in undirected graphs when they are complete, and which turns out to be comparably rare in complex unit gain graphs. The applied approach is twofold. Through an interesting parallel to various systems of lines in complex space, that equates such two-eigenvalue gain graphs with equal-norm tight frames, we provide an algebraically oriented classification of two-eigenvalue gain graphs whose least multiplicity is at most three. Moreover, various other examples stemming from well-known combinatorial objects such as the Coxeter-Todd lattice are discussed, as well as a technique that is parallel to the dismantling of association schemes, which is used to find many two-eigenvalue gain subgraphs.

Afterwards, we take a combinatorial perspective, to classify two-eigenvalue gain graphs of bounded degree. For gain graphs of degree at most four, we are able to completely characterize the collection of desired unit gain graphs. Some of these collections have infinitely many switching-distinct members, for given order and degree.

1.9 Disclosure

This thesis is based on the following five research papers. Each paper contains ideas and contributions from its respective authors.

Chapter 2	Wissing, P., & Van Dam, E. R. (2020). The negative tetrahedron and the first infinite family of connected digraphs that are strongly determined by the Hermitian spectrum. *Journal of Combinatorial Theory*, Series A, 173, 105232.
Chapter 3	Wissing, P. (2022). Self-converse mixed graphs are extremely rare. *Discrete Mathematics*, 345(10), 112989.
Chapter 4	Wissing, P., & Van Dam, E. R. (2022). Spectral fundamentals and characterizations of signed directed graphs. *Journal of Combinatorial Theory, Series A*, 187, 105573.
Chapters 5 & 7	Wissing, P., & Van Dam, E. R. (2022). Unit gain graphs with two distinct eigenvalues and systems of lines in complex space. *Discrete Mathematics*, 345(6), 112827.
Chapter 6	Wissing, P., & Van Dam, E. R. (2022). Symmetry in complex unit gain graphs and their spectra. *Work in Progress.*

CHAPTER 2

Digraphs that are strongly determined by the Hermitian spectrum

Abstract

Thus far, digraphs that are uniquely determined by their Hermitian spectra have proven elusive. Instead, researchers have turned to spectral determination of classes of switching equivalent digraphs, rather than individual digraphs. In this chapter, we consider the traditional notion: a digraph is said to be strongly determined by its Hermitian spectrum (abbreviated SHDS) if it is isomorphic to each digraph to which it is cospectral. Convincing numerical evidence to support the claim that this property is extremely rare is provided. Nonetheless, the first infinite family of connected digraphs that is SHDS is constructed. This family is obtained via the introduction of twin vertices into a structure that is named *negative tetrahedron*. This special digraph, that exhibits extreme spectral behavior, is contained in the surprisingly small collection of all digraphs with exactly one negative eigenvalue, which is determined as an intermediate result.

2.1 Introduction

While there are various matrices that may be used to describe a directed graph, there is still no consensus as to which of them best represents the characteristics of a digraph in its eigenvalues. This may be considered part of the reason that relatively well understood questions concerning undirected graphs remain wide open in the directed graph paradigm. This chapter discusses a relatively recent candidate: the Hermitian adjacency matrix [76, 51]. Of particular concern is the question: can we determine a directed graph by its Hermitian spectrum.

Being an interesting candidate for the representation of digraphs, the Hermitian adjacency matrix and its spectrum have been the subject of several recent publications. Following the two fundamental works, Mohar [83] has characterized all digraphs whose Hermitian adjacency matrix have rank 2, and shown that there are infinitely many digraphs that have cospectral mates, which are not members of the same switching equivalence class. Wang et al. [107] extends the research in [83] to the digraphs of rank 3; their main result is that any pair of weakly connected, cospectral rank 3 digraphs is switching equivalent. Although using a different approach, Tian and Wong [104] obtain similar results as in [107].

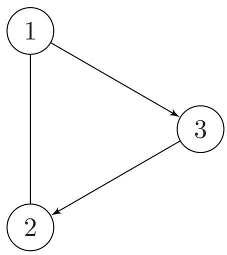
Further recent research that is concerned with the Hermitian spectrum but less relevant to the current chapter includes Greaves et al. [47], Guo and Mohar [50], Greaves [45], Hu et al. [64], Chen et al. [18] and Chen et al. [19].

Due to the presence of four-way switching, Mohar [83] defines a digraph to be determined by their H-spectrum (Abbreviated HDS hereafter) if it is cospectral only to those digraphs that are obtained from the digraph by a switching operation, possibly followed by the reversal of all edges. This definition is, however, much weaker than that of the similarly named concept in undirected graph context; if a graph G is said to be determined by its adjacency spectrum, then one is able to uniquely (up to isomorphism) construct said graph when one is given its spectrum.

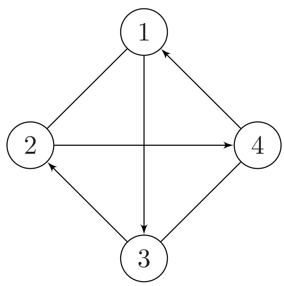
As such, the author set out to classify digraphs which are *strongly* determined by their H-spectrum; that is, digraphs whose spectra occur uniquely. Two prominent examples of such digraphs are shown in Figure 2.1. These digraphs are extremely rare, as any such digraph must be self-converse. We observe that the fraction of digraphs that satisfies this property rapidly goes to zero as the number of vertices grows. We formally show that this is in fact true in Chapter 3.

For the present chapter, the author was inspired by a result first encountered in [52] and later in [51], which occurs here as Lemma 2.7. In particular, by said lemma, there is exactly one kind of induced subdigraph of order 3 that may contribute negatively to tr $\left(H(D)^3\right)$, where $H(D)$ is the Hermitian of a digraph D. This order 3 digraph is named *negative triangle* and shown in Figure 2.1a. Furthermore, eigenvalue interlacing is used extensively.

The main results of this chapter are as follows. We construct the first infinite family of connected, strongly HDS digraphs, in Theorem 2.23. This family is obtained by twin expansion (see Def. 2.7) of a key digraph, which is named the *negative tetrahedron.* This peculiar digraph is a tetrahedron, whose four faces are all negative triangles, as is shown in Figure 2.1b. Moreover, it is the only reduced[1] digraph that has rank 4 and exactly one negative eigenvalue. Additionally, we determine all digraphs that have precisely one negative eigenvalue in Theorem 2.20, and show that any pair of connected rank 4 members of this class is switching equivalent if they are cospectral in Proposition 2.27.



(a) The negative triangle T^-



(b) The negative tetrahedron K^-

Figure 2.1 – Two strongly HDS digraphs.

2.2 Preliminaries

For an outline of the applied terminology and notation, the reader is referred to Section 1.1. Throughout this chapter, the rank and the spectral radius of a digraph are respectively the rank and the spectral radius of its Hermitian adjacency matrix. Below, a few more chapter-specific prerequisites are included.

[1] A digraph is said to be reduced if it contains no two vertices whose neighborhoods exactly coincide, and no isolated vertices. See Def. 2.5.

2.2.1 Determined by the Hermitian spectrum

As was briefly mentioned before, Mohar [83] pioneered spectral characterization with respect to the Hermitian adjacency matrix. We include the details of Mohar's definitions below.

Definition 2.1. *[83] A digraph is said to be (weakly) determined by its Hermitian spectrum (WHDS) if it is switching equivalent (see Definition 1.5) to every digraph to which it is H-cospectral.*

However, the following definition of spectral determination is in a sense more loyal to its undirected graph analogue.

Definition 2.2. *A digraph is said to be strongly determined by its Hermitian spectrum (SHDS) if it is isomorphic to every digraph to which it is H-cospectral.*

The distinction between Definitions 2.1 and 2.2 summarizes what sets this work apart from previous articles regarding Hermitian spectral characterization. To distinguish between the two definitions, the author has added the word "weakly" to the former and "strongly" to the latter. The terminology is justified by the observation that any SHDS digraph is implicitly WHDS.

We end this section with a few words of warning, regarding a frequent mistake surrounding the term (W)HDS. Since neither four-way switching nor taking the converse changes a digraph's underlying graph, two digraphs of which just one is connected cannot be switching equivalent. Hence, if a connected digraph is cospectral to a digraph that contains isolated vertices, neither may be said to be (W)HDS. While [107, 104] show that any pair of cospectral, connected rank 3 digraphs is switching equivalent, cases in which such a connected digraph is cospectral to a disconnected digraph may still be found. Therefore, the phrasing of the final theorems of both [107] and [104], in which it is claimed that any rank 3 digraph is (W)HDS, is flawed.

2.2.2 Known results

Here, we will list some of the results that are vital to the discussion in this paper. Likely the single most used tool throughout is known as eigenvalue interlacing, which is a particularly powerful tool, adopted from graph theory. In particular, Lemma 1.1 will be one of the tools to determine the collection of all digraphs with a single negative eigenvalue. To explicitly write the spectra of these families, the concepts known as *quotient matrix* and *equitable partition* are used. Both originate from [55], in graph context, and have been published in [51] for Hermitian context.

Let D be a digraph and let $\mathcal{V} = \{V_1, \dots, V_k\}$ be a partition of $V(D)$. One may order the vertices of V such that $\mathcal{V}$ induces a partition of H into block matrices as

$$H = \begin{bmatrix} H_{11} & \cdots & H_{1k} \\ \vdots & \ddots & \vdots \\ H_{k1} & \cdots & H_{kk} \end{bmatrix}.$$

The quotient matrix of a Hermitian H with respect to $\mathcal{V}$ is the matrix $Q = [q_{ij}]$, $i, j \in [k]$, where q_{ij} is the average row sum of block H_{ij}. The partition $\mathcal{V}$ is said to be *equitable* if every block H_{ij} has constant row sum. One then has the following result.

Lemma 2.1. *[51] Let D be a digraph with Hermitian H, and let $\mathcal{V}$ be an equitable partition of its vertices. Moreover, let Q be the quotient matrix of H with respect to $\mathcal{V}$. If λ is an eigenvalue of Q with multiplicity μ, then it is an eigenvalue of H with multiplicity at least μ.*

In [83], Mohar works with digraphs of rank 2, particularly those that are complete bipartite or complete tripartite. With regard to the former, the following unproven claim is made.

Conjecture 1. *[83] There are only finitely many integers m and n for which the complete bipartite graph $K_{m,n}$ is WHDS.*

Regarding complete tripartite digraphs, Mohar claims that there are many instances that are WHDS for number theoretic reasons. In particular, if we denote by $\overrightarrow{C}_3(a, b, c)$ the complete tripartite digraph with parts A, B, C, where $|A| = a$, $|B| = b$ and $|C| = c$, with all arcs from A to B, B to C, and C to A, then the following claims hold.

Proposition 2.2. *[83] $\overrightarrow{C}_3(n, n, n)$, $\overrightarrow{C}_3(n, n, n + 1)$ and $\overrightarrow{C}_3(n - 1, n, n)$ are WHDS for every n.*

Corollary 2.2.1. *[83] Suppose that a and $n > a > 0$ are integers such that $a^2 < 2n$. Then $\overrightarrow{C}_3(n - a, n, n + a)$ is WHDS if and only if a is not divisible by a prime that is congruent to 1 modulo 6.*

This line of research was extended to rank 3 independently by Wang et al. [107] and Tian and Wong [104]. Of most relevance to this work is the following result.[2]

Proposition 2.3. *[107, 104] Any two connected, cospectral, rank* 3 *digraphs are switching equivalent.*

However, Wang et al. [107] also show that, if the assumption on connectedness is omitted, one may construct infinite families of rank 3 digraphs that are not WHDS.

Proposition 2.4. *[107] There are infinitely many digraphs with rank* 3 *that are not WHDS.*

2.2.3 Twins

The first half of the discussion in this chapter will concern 'small' digraphs with exactly one negative eigenvalue; the second half will extend this discussion to 'large' digraphs. That said, the discussed digraphs remain largely similar, from a structural point of view. Specifically, in order to increase the size of the considered digraphs without compromising the structural arguments made in the former part, *twins* are introduced into the small digraphs. Since there have been several authors (e.g., [3, 14]) to have introduced a similarly named concept, each with subtle differences, we provide the formal definition as it is used throughout this paper.

Definition 2.3. *Two vertices u, v in D, whose Hermitian is H, are called twins if $H_{ux} = H_{vx}$ for every $x \in V(D)$.*

A simple but important observation is that u and v are implicitly not twins if $H_{uv} \neq 0$, as loops are not allowed throughout. Moreover, if u, v, w are vertices in D, w is said to *distinguish* u and v if $H_{uw} \neq H_{vw}$. Naturally, if such a vertex w exists in D, then u and v are not twins in D, which justifies the terminology.

We will often want to consider the structure that is in a sense fundamental to a large digraph that contains a set of equivalent vertices. To this end, we define the *twin reduction* operation, which reduces such a collection of twin vertices down to a single vertex; this may significantly reduce the order of a digraph, while retaining its general structure and rank. Moreover, using said operation, we define a property that characterizes digraphs we consider to be 'small'.

[2]Originally formulated as *"All connected digraphs of order n with rank* 3 *are WHDS,"* which is not entirely accurate, as discussed at the end of Sec. 1.1. The author took the liberty of slightly rephrasing to avoid confusion.

Definition 2.4. *We define $TR(\cdot)$ to be the twin reduction operator, which removes vertices and edges from a digraph in such a way that exactly one of every collection of twins is kept and no isolated vertices remain.*

Definition 2.5. *A digraph D is called reduced if $TR(D) = D$.*

Naturally, we may also want to reverse this operation, to increase the size of the digraph without compromising the fundamental structure. The formal definition of the corresponding operation is given below.

Definition 2.6. *A vector $t = \begin{bmatrix} t_0 & t_1 & \cdots & t_n \end{bmatrix} \in \mathbb{N}_0^n$ is called an expansion vector for a digraph D if $n = |V(D)|$ and $t_1, \ldots, t_n \geq 1$.*

Definition 2.7. *Let D be a digraph with an ordered set V of n vertices, and let t be an appropriate expansion vector. The twin expansion of D with respect to t is denoted $D' = TE(D, t)$ and is obtained by replacing each vertex u in D by t_u twins, and adding t_0 isolated vertices. Formally, if $V = [n]$, let $V(D') = V_0 \cup V_1 \cup \cdots \cup V_n$, where $V_0, V_1, \ldots, V_n$ are mutually disjoint sets, with $|V_u| = t_u$. In D', V_0 is a set of isolated vertices, and $H'_{u'v'} = H_{uv}$ for every $u' \in V_u$, $v' \in V_v$, $u, v \in V$, where H and H' are the Hermitians of D and D', respectively.*

Note that each entry of the expansion vector thus corresponds to a specific vertex in the digraph that is to be expanded. As a direct consequence, the vertex ordering does matter, in the sense that permuting the expansion vector does not change the resulting (expanded) digraph if the vertex order of the source digraph is permuted accordingly. Thus, we will fix the vertex orderings of the relevant digraphs to ensure that the above does not occur, when permutations of given expansion vectors are discussed. Specifically, this ordering is given by the vertex labels of the defining illustrations.

For the sake of clarity, we include the following example that shows the working of the twin expansion operator.

Example 2.1. *Let $t = \begin{bmatrix} 2 & 3 & 2 & 1 \end{bmatrix}$. Then the vertices of the negative triangle T^-, shown in Figure 2.1a, and its twin expansion $D' = TE(T^-, t)$ may be labeled such* *that their Hermitians are*

$$H(T^-) = \begin{bmatrix} 0 & 1 & i \\ 1 & 0 & -i \\ -i & i & 0 \end{bmatrix} \text{ and } H(D') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & i \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & i \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & i \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & -i \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & -i \\ 0 & 0 & -i & -i & -i & i & i & 0 \end{bmatrix}.$$

We conclude this section with two observations that will be quite obvious to the experienced graph theorist, though the ideas are in a sense key to the presented discussion. As such, their proofs are omitted.

Lemma 2.5. *Let D be a digraph of order n and let t be an expansion vector for D. Then*

$$\text{Rank } H(TR(D)) = \text{Rank } H(D) = \text{Rank } H(TE(D,t)) \tag{2.1}$$

Lemma 2.6. *Let D be a digraph of order n and let t be an expansion vector for D. Suppose that D has p positive and q negative eigenvalues. Then $TE(D,t)$ and $TR(D)$ also have p positive and q negative eigenvalues.*

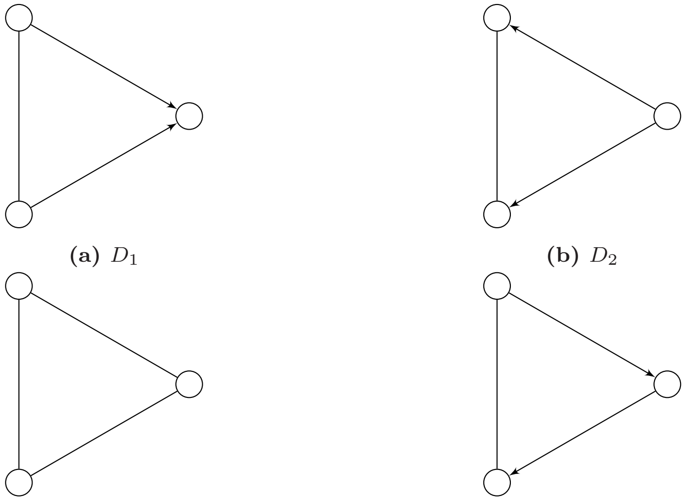
2.3 The negative tetrahedron

In the present paper, we are interested in families of digraphs that contain many copies of a given substructure, which is in a sense counted by the spectrum. In this section, we will provide a thorough introduction of these families and the elementary observations upon which many of the later results are built.

2.3.1 Digraphs related to the negative triangle

Upon investigation of properties that may be inferred from the Hermitian spectrum of a digraph, we are inspired by the following lemma by Guo [52], that ties in closely to a similar, well-known result for undirected graphs (see Brouwer and Haemers [11]).

Lemma 2.7. *[52] Let D be a digraph with Hermitian H. Then $tr\left(H^3\right) = 6(x_1 + x_2 + x_3 - x_4)$, where x_j denotes the number of copies of D_j that occur as induced subdigraphs of D. The structures $D_1, \ldots, D_4$ are shown in Figure 2.2.*



(a) D_1 (b) D_2

(c) D_3 (d) D_4

Figure 2.2 – The four triangles that conribute to tr $\left(H^3\right)$.

The main observation to take away from Lemma 2.7 is that apparently, the structure D_4, above, is the only order 3 substructure that has a negative impact on tr $\left(H^3\right)$, which in turn may be computed directly from the spectrum of a digraph. Thus, we may be able to identify (or even determine) digraphs that have many such substructures. In the interest of clearness, we name the following two structures, which occurred before in Figure 2.1 and that are in a sense fundamental to the discussion in this paper.

Definition 2.8. *Figure 2.2d is called the negative triangle and is denoted T^-.*

Definition 2.9. *Figure 2.3 is called the negative tetrahedron and is denoted K^-.*

The negative tetrahedron is an interesting digraph for a number of reasons, and has come up in the before mentioned works. One might first notice its extreme degree of structural symmetry; K^- is, in fact, vertex-transitive. A second interesting fact is that T^- and K^- are exactly the two digraphs with rank more than 2 that are antispectral[3] to a complete graph. T^- and K^-, whose spectra are $\{-2, 1^{[2]}\}$ and $\{-3, 1^{[3]}\}$, respectively, are antispectral to respectively K_3 and K_4. Guo and Mohar [51] have shown that there are no higher rank digraphs that admit to this property.

[3] A pair of digraphs D and D' is said to be *antispectral* to one another if $\Sigma_D = -\Sigma_{D'}$.

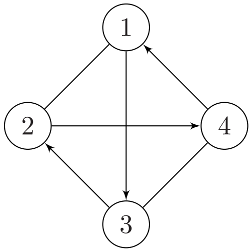
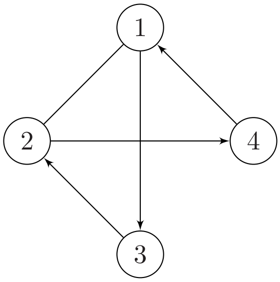
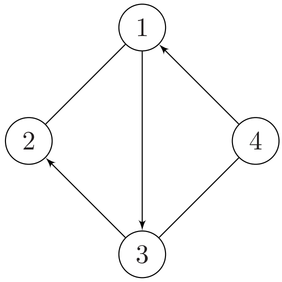


Figure 2.3 – The negative tetrahedron K^{-}.



(a) T_a^{-}



(b) T_b^{-}

Figure 2.4 – Illustrations for Def. 2.10.

Lastly, it is mentioned in [51] that K^{-} exhibits extreme spectral behavior, in the sense that it attains the bound $\rho(D) \leq 3\mu_1$, where μ_1 is the largest eigenvalue of D.

In addition to T^{-} and K^{-}, there are two more digraphs that play a prominent role throughout this paper. In the interest of structure, we include their definitions here.

Definition 2.10. *The digraphs T_a^{-} and T_b^{-} are shown in Figures 2.4a and 2.4b, respectively.*

We note that both digraphs are reduced and have rank 3. Furthermore, we observe that T_a^{-} and T_b^{-} are closely related to T^{-}, from a spectral point of view. In fact, if one expands a single vertex of T^{-} once (to obtain, say, $T_{1,1,2}^{-}$), then $T_{1,1,2}^{-}$, T_a^{-}, T_b^{-} are all cospectral and switching equivalent. More detail concerning this relation is provided at the end of Section 2.3.3.

2.3.2 The first families of SHDS digraphs

Using only the tools we have thus far, we are already able to construct some infinite SHDS families. Probably the first, most trivial SHDS digraph that comes to mind is the empty graph of order p, denoted O_p. Indeed, using that $2|E(\Gamma(O_p))| = \operatorname{tr}\left(H(O_p)^2\right) = 0$, the all-zero spectrum certainly determines the empty graph.

It is easy to check that T^- is the smallest non-empty digraph that is strongly determined by its Hermitian spectrum. In fact, it is a simple exercise to show the following result,[4] that signifies the essential role T^- and K^- play in the proposed discussion. As a first step towards a less trivial infinite family of SHDS digraphs, we classify all digraphs with largest eigenvalue 1.

Lemma 2.8. *Let D be a connected digraph with largest eigenvalue* 1*. Then D is either K_2, K_2', T^-, or K^-, where K_2' is the oriented K_2.*

Proof. By interlacing, it follows that there is no $U \subseteq V(D)$ such that $\Gamma(D[U]) = P_3$, since every digraph whose underlying graph is P_3 has $\mu_1 = \sqrt{2}$, where μ_1 is the largest eigenvalue. Hence, $\Gamma(D) = K_n$, for $n \in \mathbb{N}$. If $n = 2$, both digraphs D with $\Gamma(D) = K_2$ have $\mu_1 = 1$, and are therefore valid options. Note that $n = 3$, $\mu_1 = 1$ only if $D = T^-$; other potential digraphs of order 3 have an eigenvalue $\sqrt{3}$ or 2. Moreover, one should also observe that if $n > 3$, each order-3 induced subdigraph of D should again be T^-, or else the claim is false by interlacing. Thus, if $n = 4$, $D = K^-$. Moreover, as before, if $n > 4$, any order 4 induced subdigraph of D must be K^-.

Finally, suppose that $n \geq 5$, and suppose that $D[\{1, 2, 3, 4\}] = D[\{1, 2, 3, 5\}] = K^-$. (Note that we are not imposing any extra assumptions; if these induced subdigraphs are not K^-, D certainly has $\mu_1 > 1$.) Then we have $D[\{1, 4, 5\}] \neq T^-$, as $H(D)_{1,4} = H(D)_{1,5}$. It follows that $\mu_1 > 1$, by which we have a contradiction and thus $n \leq 4$. $\square$

By the result above, we are able to draw an interesting conclusion with regard to the spectral determination of the class of digraphs with largest eigenvalue 1.

Corollary 2.8.1. *Let D be a digraph with largest eigenvalue* 1*. Then D is WHDS.*

Proof. By Lemma 2.8, every connected component must be K_2, K_2', T^-, or K^-. It should be clear that every eigenvalue -3 belongs to a copy of K^-, every eigenvalue

[4] A similar result occurs as Prop. 5.2 in [51], which concerns digraphs antispectral to K_n. While the obtained collection of digraphs is almost identical, the author chose to include a proof as the claim requirements and the argument are signifficantly different.

-2 belongs to a T^-, and every eigenvalue 0 belongs to an isolated node. Likewise, every eigenvalue -1 belongs to K_2 or K_2'. Since K_2 is clearly switching equivalent to K_2', the claim follows. □

Moreover, if one excludes K_2 and K_2', such a digraph is SHDS, by the same argument.

Corollary 2.8.2. *Let D be a digraph with largest eigenvalue 1 and no eigenvalues -1. Then D is SHDS.*

Thus, we have obtained an infinite family of SHDS digraphs, that may consist of arbitrarily many disjoint copies of T^- and K^-, as well as isolated vertices.

2.3.3 The spectra of expansions of K^- and related digraphs

In the discussion leading up to our main theorem, we will be interested in twin expansions (recall Def. 2.7) of K^-, in particular. The following Lemma is added for completeness; its correctness should be evident from a brief look at Figure 2.5.

Lemma 2.9. *Let $t = \begin{bmatrix} t_0 & t_1 & t_2 & t_3 & t_4 \end{bmatrix}$ and let $D_t = TE(K^-, t)$. Then D_t contains $n = \sum_{i=0}^{4} t_i$ vertices, $m = \sum_{1 \leq i < j \leq 4} t_i t_j$ edges, and $k = \sum_{1 \leq i < j < l \leq 4} t_i t_j t_l$ copies of T^-.*

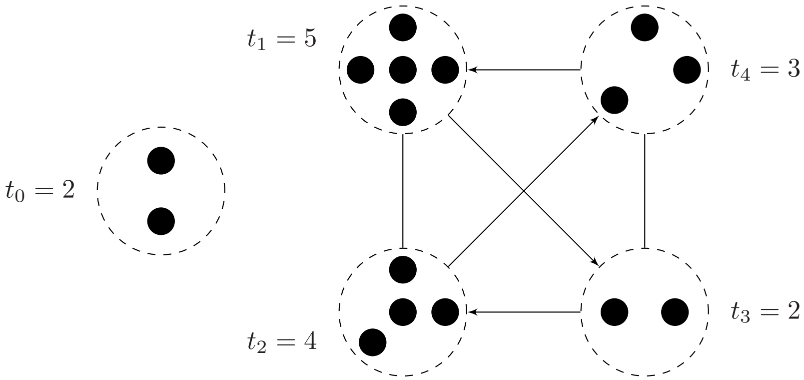


Figure 2.5 – A digraph obtained as $TE\left(K^-, [2\ 5\ 4\ 2\ 3]\right)$. Here, the dashed circles indicate clusters of twins and an edge between two clusters is used to draw all edges of that type between the members of said clusters.

Note that a permutation of the coefficients $t_1, \ldots, t_4$ would not necessarily yield an isomorphic digraph, as is illustrated in Example 2.3, (Sec. 2.5) while the spectrum is invariant under such a permutation, as we will see shortly.

As we set out to show that particular twin expansions of K^- are SHDS, it seems fitting to include the explicit spectra of this interesting family of digraphs. In the below, we write their characteristic polynomials explicitly by employing Lemma 2.1. While one could have used a before-mentioned result from [76] that counts elementary subdigraphs to obtain the coefficients in (2.2), the author found the approach below to be significantly more comprehensible.

Lemma 2.10. *Let* $t = \begin{bmatrix} t_0 & t_1 & t_2 & t_3 & t_4 \end{bmatrix}$ *be an expansion vector and let* $n = \sum_{i=0}^{4} t_i$. *Then* $D = TE(K^-, t)$ *has characteristic polynomial*

$$\chi_D(\mu) = \mu^{n-4}\left(\mu^4 - \left(\sum_{1\le i<j\le 4} t_i t_j\right)\mu^2 + 2\left(\sum_{1\le i<j<k\le 4} t_i t_j t_k\right)\mu - 3\prod_{i=1}^{4} t_i\right). \tag{2.2}$$

Proof. By construction, we may write the Hermitian of D as the block matrix

$$H(TE(K^-,t)) = \begin{bmatrix} 0 & 0 \\ 0 & M \end{bmatrix}, \text{ where } M = \begin{bmatrix} 0 & J & iJ & -iJ \\ J & 0 & -iJ & iJ \\ -iJ & iJ & 0 & J \\ iJ & -iJ & J & 0 \end{bmatrix}, \tag{2.3}$$

where the diagonal blocks have sizes $t_0 \times t_0, \ldots, t_4 \times t_4$, respectively. Note that all of the blocks in (2.3) are constant, and thus (2.3) is a so-called equitable partition. We may then write the 4×4 quotient matrix [55, 51] B as

$$B = \begin{bmatrix} 0 & t_2 & it_3 & -it_4 \\ t_1 & 0 & -it_3 & it_4 \\ -it_1 & it_2 & 0 & t_4 \\ it_1 & -it_2 & t_3 & 0 \end{bmatrix}.$$

One may compute $\det(\mu I - B)$ to find

$$\chi_B(\mu) = \mu^4 - \left(\sum_{1\le i<j\le 4} t_i t_j\right)\mu^2 + 2\left(\sum_{1\le i<j<k\le 4} t_i t_j t_k\right)\mu - 3\prod_{i=1}^{4} t_i.$$

Now, observe that Rank $(B) = 4$. Hence, $\chi_B(\mu)$ has four nonzero roots, which are the (not necessarily distinct) eigenvalues $\lambda_1, \ldots, \lambda_4$ of B. Since (2.3) is an equitable partition, each of the λ_j also occur as an eigenvalue of $H(TE(K^-, t))$. Moreover, since by construction Rank $(H(TE(K^-, t))) = \text{Rank}\,(B) = 4$, it is clear that we have

$$\begin{aligned}\chi_D(\mu) &= \mu^{n-4}(\mu - \lambda_1)(\mu - \lambda_2)(\mu - \lambda_3)(\mu - \lambda_4)\\ &= \mu^{n-4}\chi_B(\mu).\end{aligned}$$

□

Moreover, by plugging in t, one may readily show the following results.

Corollary 2.10.1. *Let $t_1, t_2, t_3 \in \mathbb{N}$ and $t_0 \in \mathbb{N}_0$. For the following special cases of expansion vector t, we may write the spectrum of $D = TE(K^-, t)$ explicitly. In the below, n is the sum of the entries of t.*

(i) If $t = \begin{bmatrix} t_0 & t_1 & t_1 & t_1 & t_1 \end{bmatrix}$ *then*

$$\Sigma_D = \left\{-3t_1, t_1^{[3]}, 0^{[n-4]}\right\}.$$

(ii) If $t = \begin{bmatrix} t_0 & t_1 & t_1 & t_1 & t_2 \end{bmatrix}$ *then*

$$\Sigma_D = \left\{-t_1 - \sqrt{3t_1t_2 + t_1^2}, \quad -t_1 + \sqrt{3t_1t_2 + t_1^2}, \quad t_1^{[2]}, \quad 0^{[n-4]}\right\}.$$

(iii) If $t = \begin{bmatrix} t_0 & t_1 & t_1 & t_2 & t_2 \end{bmatrix}$ *then*

$$\begin{aligned}\Sigma_D = \Bigg\{ & t_1, t_2, \frac{1}{2}\left(-t_1 - t_2 + \sqrt{t_1^2 + 14t_1t_2 + t_2^2}\right),\\ & \frac{1}{2}\left(-t_1 - t_2 - \sqrt{t_1^2 + 14t_1t_2 + t_2^2}\right), 0^{[n-4]}\Bigg\}\end{aligned}$$

Proof. Follows directly by plugging t into Lemma 2.10. □

Corollary 2.10.2. *Let $t_1, t_2, t_3 \in \mathbb{N}$ and $t_0 \in \mathbb{N}_0$. If $t = \begin{bmatrix} t_0 & t_1 & t_1 & t_2 & t_3 \end{bmatrix}$ then $TE(K^-, t)$ has an eigenvalue t_1.*

Proof. Plug in (2.2) to find

$$\chi_D(\mu) = \mu^{n-4}(\mu - t_1)(\mu^3 + t_1\mu^2 - (2t_1t_2 + 2t_1t_3 + t_2t_3)\mu + 3t_1t_2t_3),$$

which clearly has a root at $\mu = t_1$. □

Now, one would like to conclude that the reverse is also true; that from the occurrence of an integer eigenvalue μ_j it follows that an expansion vector contains μ_j twice. This is in general not true, as shown by the following example.

Example 2.2. *Suppose that* $t = \begin{bmatrix} 0 & 1 & 2 & 6 & 9 \end{bmatrix}$. *Then, by Lemma 2.10,* $D = TE(K^-, t)$ *has characteristic polynomial*

$$\chi_D(\mu) = \mu^{14}\left(\mu^4 - 101\mu^2 + 384\mu - 324\right) = \mu^{14}(\mu - 3)(\mu^3 + 3\mu^2 - 92\mu + 108),$$

and thus D *has an eigenvalue* 3, *while none of the* t_i *equals* 3.

That said, if an integer eigenvalue μ_j occurs at least twice, then we are able to conclude the reverse, as we will discuss in the proof of Theorem 2.23.

We conclude this section with some brief notes regarding the spectral similarity of T^-, T_a^-, and T_b^-, and their respective expanded versions. As before, we are able to compute their spectra explicitly by employing the quotient matrix.

Lemma 2.11. *Let* $t = \begin{bmatrix} t_0 & t_1 & t_2 & t_3 \end{bmatrix}$ *be an expansion vector and let* $n = \sum_i t_i$. *Then* $D = TE(T^-, t)$ *has characteristic polynomial*

$$\chi_D(\mu) = \mu^{n-3}\left(\mu^3 - (t_1t_2 + t_1t_3 + t_2t_3)\mu + 2t_1t_2t_3\right).$$

Lemma 2.12. *Let* $t = \begin{bmatrix} t_0 & t_1 & t_2 & t_3 & t_4 \end{bmatrix}$ *and be an expansion vector. Let* $D'_a = TE(T_a^-, t)$ *and* $D'_b = TE(T_b^-, t)$. *Then*

$$\chi_{D'_a}(\mu) = \mu^{n-3}\left(\mu^3 - (t_1t_2 + t_1(t_3 + t_4) + t_2(t_3 + t_4))\mu + 2t_1t_2(t_3 + t_4)\right)$$

and

$$\chi_{D'_b}(\mu) = \mu^{n-3}\left(\mu^3 - (t_1t_3 + t_1(t_2 + t_4) + t_3(t_2 + t_4))\mu + 2t_1t_3(t_2 + t_4)\right).$$

Thus, it follows that $TE(T^-, \begin{bmatrix} t_0 & t_1 & t_2 & (t_3 + t_4) \end{bmatrix})$, $TE(T_a^-, \begin{bmatrix} t_0 & t_1 & t_2 & t_3 & t_4 \end{bmatrix})$

and $TE(T_b^-, \begin{bmatrix} t_0 & t_1 & t_3 & t_2 & t_4 \end{bmatrix})$ are all cospectral. Lastly, note that these digraphs are also all pairwise switching equivalent.

2.4 Classification of digraphs with one negative eigenvalue

In order to construct the desired infinite family of SHDS digraphs, we first set out to find its smallest members. It turns out that the members of the family in which we are interested share the interesting property of only having a single negative eigenvalue; a property that is satisfied by very few reduced digraphs. We note the following useful observation with regard to such digraphs.

Lemma 2.13. *Let D be reduced with exactly one negative eigenvalue. Then D is connected.*

Proof. Note that the spectrum of any connected component of order at least 2 contains at least one negative eigenvalue, since the sum of the eigenvalues of a Hermitian matrix must sum up to its trace, which is zero for the Hermitian adjacency matrix of a digraph without loops. Moreover, recall that if D consists of two disjoint, connected components D_1 and D_2, then $\Sigma_D = \Sigma_{D_1} \cup \Sigma_{D_2}$, and thus Σ_D contains at least two negative elements. Lastly, note that no isolated vertices are allowed by definition of reducedness. □

We also impose a minor assumption on the rank of the considered digraphs, in order to exclude cases that are in a sense trivial. Specifically, we require digraphs to have rank larger than 2. Recall that there are no digraphs with rank less than 2 besides the empty graph, and that any nonempty rank 2 digraph trivially has precisely one positive and one negative eigenvalue, by the observation above. However, no such digraph is interesting for the present paper, as any rank 2 digraph is cospectral to its underlying graph [83] and such digraphs are in general not WDHS.[5] As such, we exclude this class of digraphs; the interested reader is referred to [83], in which this class is researched in considerable detail.

If one requires the considered digraphs to have rank larger than 2 in addition to being reduced, one finds just four digraphs. The main result of this section, which is the following theorem, shows exactly that.

[5]By employing twin expansion on e.g., K_2 and $\overrightarrow{C}_3$, one easily finds cospectral classes whose members have at least two distinct underlying graphs.

Theorem 2.14. *Let D be a reduced digraph of rank larger than 2 and with exactly one negative eigenvalue. Then D is one of T^-, T_a^-, T_b^-, or K^-.*

In order to prove Theorem 2.14, we first show several intermediate results. First, we will provide a few crucial observations that are somewhat obvious, but that are added for the sake of completeness. In Proposition 2.16, we will see that there are exactly three reduced digraphs on four vertices that have the required single negative eigenvalue. The remainder of the section is concerned with bounding the size of a reduced digraph with exactly one negative eigenvalue. In particular, we will find that such a digraph may contain at most four vertices; the correctness of Theorem 2.14 then follows.

As was mentioned before, the negative triangle T^- plays an essential role throughout. The simple, but useful fact that any digraph of sufficient rank must contain such triangles if it has a single negative eigenvalue, is shown below.

Lemma 2.15. *Let D be a digraph with rank larger than 2. If D has a single negative eigenvalue, then $D[U] = T^-$ for some $U \subseteq V(D)$.*

Proof. Let $\lambda_1, \lambda_2, \ldots, \lambda_p$ be the p positive eigenvalues of D and let λ_n be the negative eigenvalue. We have $\lambda_n = -\sum_j^p \lambda_j$, so $\operatorname{tr}\left(H(D)^3\right) = \sum_j^p \lambda_j^3 - \left(\sum_j^p \lambda_j\right)^3 < 0$ and thus D contains at least one negative triangle by Lemma 2.7. □

Corollary 2.15.1. *If D is a digraph with order 3, rank larger than 2, and exactly one negative eigenvalue, then $D = T^-$.*

We are now ready to show the first major result, in which we obtain the collection of order four digraphs that meets our requirements. We would remark here that, while the collection of all order four digraphs is small enough to simply apply full enumeration by computer, the author opts for a constructive argument that may be used in similar fashion when the order is increased.

Proposition 2.16. *Let D be a reduced digraph with order 4, rank larger than 2, and exactly one negative eigenvalue Then D is one of T_a^-, T_b^-, or K^-.*

Proof. Let D be a digraph of order 4, with exactly one negative eigenvalue, and rank larger than 2. By Lemma 2.15, D contains T^-. Hence, we may write $H(D)$ as

$$H(D) = \begin{bmatrix} 0 & 1 & i & -i \cdot \bar{z}_1 \\ 1 & 0 & -i & i \cdot \bar{z}_2 \\ -i & i & 0 & \bar{z}_3 \\ i \cdot z_1 & -i \cdot z_2 & z_3 & 0 \end{bmatrix},$$

where $z = [z_1 \quad z_2 \quad z_3] \neq 0$, $z_j \in \{0, \pm 1, \pm i\}$ and $z_1 \neq i$, $z_2 \neq -i$, $z_3 \neq -1$. Note that the variable entries of $H(D)$ are put in this form to make (2.4) symmetric. One then readily obtains that

$$\det H(D) = \sum_{j=1}^{3} |z_j| \; - 2 \sum_{1 \leq i < j \leq 3} \operatorname{Re}(z_i \bar{z}_j). \tag{2.4}$$

Now, we make the following observation. Since D contains T^-, it has at least two positive eigenvalues, by interlacing. Moreover, from $\det H(D) = \prod_j \lambda_j$ it follows that $\det H(D) > 0$ if and only if D has an even number of negative eigenvalues. Hence, D satisfies the requirements of the claim if and only if the corresponding z is such that $\det H(D) \leq 0$. Note that if exactly one z_j is nonzero, one may plug in (2.4) to obtain $\det H(D) = 1$, and thus $H(D)$ has more than one negative eigenvalue. Therefore, at least two elements of z must be nonzero.

Suppose that two elements of z are nonzero. Then $\det H(D) \geq 0$ (by (2.4)) and thus we are only interested in the case that $\det H(D) = 0$. Suppose that $z_3 = 0$. Then $\det H(D) = 0 \iff |z_1| + |z_2| = 2\operatorname{Re}(z_1 \bar{z}_2) \iff z_1 \bar{z}_2 = 1 \iff z_1 = z_2$. Hence, either $z = \begin{bmatrix} 1 & 1 & 0 \end{bmatrix}$ or $z = \begin{bmatrix} -1 & -1 & 0 \end{bmatrix}$. Similarly, if $z_2 = 0$ then $z = \begin{bmatrix} 1 & 0 & 1 \end{bmatrix}$ or $z = \begin{bmatrix} -i & 0 & -i \end{bmatrix}$ and if $z_1 = 0$ then $z = \begin{bmatrix} 0 & 1 & 1 \end{bmatrix}$ or $z = \begin{bmatrix} 0 & i & i \end{bmatrix}$. It is readily verified that out of these six possible z, three correspond to a digraph that contains a twin and therefore do not meet the requirements of the claim; the remaining three z correspond to either T_a^- or T_b^-.

Lastly, suppose that no element of z is zero. It is easily observed from (2.4) that $\det H(D) \neq 0$, since $\operatorname{Re}(z_i \bar{z}_j) \in \mathbb{Z}\ \forall i, j$ and $3 = 2(m_1 + m_2 + m_3)$ has no solution for $m_1, m_2, m_3 \in \mathbb{Z}$. Thus, any z that meets the requirements of the claim has $\det H(D) < 0$. Hence, $\operatorname{Re}(z_i \bar{z}_j) \geq 0\ \forall i, j$, with at most one pair (i, j) such that $\operatorname{Re}(z_i \bar{z}_j) = 0$. W.l.o.g., assume that $z_1 \bar{z}_2 = z_1 \bar{z}_3 = 1$. Then $z_1 = z_2$ and $z_1 = z_3$, and thus $z = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$, which corresponds to exactly K^-. $\square$

In order for us to prove Theorem 2.14, we should consider the reduced digraphs of larger order. As we will shortly show, we find that no digraph of order larger than 4 satisfies both required properties, i.e., being reduced and having exactly one negative eigenvalue. In the interest of structure, the discussion to support this claim is split up into Lemmas 2.17, 2.18 and 2.19.

The approach below is, for the most part, based on the idea of taking some small substructure that is certainly contained in any of the candidates, and attempting to build a digraph that meets all requirements by adding vertices and edges to it. In particular, all of the digraphs we encounter contain at least one copy of T^-. Moreover, from the results at the top of this section, we know that there are scarcely any ways to extend T^- with vertices and edges without invalidating assumptions. Using these facts, we will show in Lemmas 2.17, 2.18 and 2.19 that the order of the digraphs that have so far been shown to satisfy our requirements cannot be extended without introducing a twin vertex.

Lemma 2.17. *Suppose that D is a digraph of order $n \geq 4$, rank larger than 2, that does not contain T_a^-, T_b^-, or K^-. Moreover, suppose that D has exactly one negative eigenvalue. Then D is not reduced.*

Proof. By contradiction. We will show, through combinatorial reasoning, that a digraph that admits to the assumptions in the claim must contain twins. This reasoning is illustrated with an example in Figure 2.6. We note that while the exact nature of the edges in Figure 2.6 may differ depending on u, the reasoning below remains valid.[6]

Suppose that D is reduced. By Lemma 2.15, D contains T^- as an induced subdigraph and D is connected by Lemma 2.13. Let $U \subset V(D)$ be such that $D[U] = T^-$. As $n \geq 4$, there must be a vertex $v \in v(D)$ that is adjacent to U in D. We now observe that $D[U \cup \{v\}]$ must contain a twin. Indeed, if we suppose that $D[U \cup \{v\}]$ is reduced, then by Proposition 2.16, $D[U \cup \{v\}]$ is either T_a^-, T_b^- or K^-. However, since none of these digraphs are allowed to be contained as induced subdigraphs, by the requirements of the claim, we have a contradiction. Thus, $D[U \cup \{v\}]$ is not reduced, and v is the twin of a vertex $u \in U$ in $D[U \cup \{v\}]$. (At this point, $D[U \cup \{v\}]$ may look like Figure 2.6a.)

[6]In fact, one could even disregard the arc orientations in Figure 2.6 altogether and apply the reasoning in the proof of Lemma 2.17 to the underlying graph of the considered digraph, without compromising the proof. The author has opted for an example that best illustrates the situation at hand.

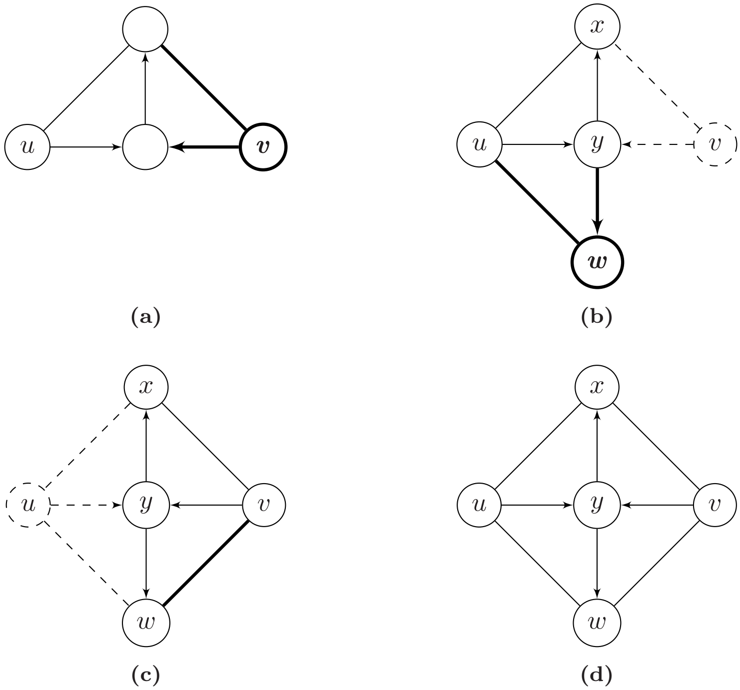


Figure 2.6 – Illustration for the proof of Lemma 2.17. Bold elements indicate the most recent additions to the structure; dashed elements are temporarily ignored.

But since D is assumed to be reduced, there must be some vertex that distinguishes u from v in D. Let us call this vertex w and assume without loss of generality that w is adjacent to u. Then, consider $D[U \cup \{w\}]$ and use the same argument as above to obtain that w must be the twin of some vertex $x \in U \setminus \{u\}$ (since u and w are adjacent) in $D[U \cup \{w\}]$. Label the final unlabeled vertex in U with y; we then obtain Figure 2.6b. Note that, again, by the same argument, $D[\{v, w, x, y\}]$ contains T^- and should thus contain a twin. But as w is not adjacent to x (since w is the twin of x in $D[\{u, w, x, y\}]$), w must be adjacent to v and implicitly w is the twin of x in $D[\{v, w, x, y\}]$ as well, (Figure 2.6c) and hence also in $D[\{u, v, w, x, y\}]$. Finally, if we consider the full structure (Figure 2.6d) it then follows that w does not distinguish between u and v, which is a contradiction. $\square$

Let us now consider digraphs that do contain T_a^-, T_b^-, or K^-.

Lemma 2.18. *Suppose that D is a digraph of order $n = 5$, that contains T_a^-, T_b^-, or K^-. Moreover, suppose that D has exactly one negative eigenvalue. Then D is not reduced.*

Proof. First, suppose that $U \subset V(D)$ is such that $D[U] \cong K^-$. Let v be the fifth vertex in $V(D)$. We may assume that v is not an isolated vertex, otherwise D would not be reduced. We make the following observations from Proposition 2.16: v cannot have valency 1, and if v has valency 3, then the subdigraph of D induced by v and its neighbors is isomorphic to K^-. It then follows that v is connected to at least two out of every three vertices in U. This, in turn, implies that v has valency at least 3.

Suppose that v has valency 3, let $u \in U$ be non-adjacent to v and let $U' = U \setminus \{u\} \cup \{v\}$. Then $D[U'] \cong K^-$, and thus it follows that u and v are twins. If v has valency 4, one may apply the same argument twice to obtain that v should be the twin of two distinct vertices in U, which is impossible. Hence, v has valency 3 and D is not reduced.

Next, suppose that $D[U] \cong T_a^-$. Then one may write

$$\det H(D) = \det \begin{bmatrix} 0 & 1 & i & -i & -i \cdot \bar{z}_1 \\ 1 & 0 & -i & i & i \cdot \bar{z}_2 \\ -i & i & 0 & 0 & \bar{z}_3 \\ i & -i & 0 & 0 & \bar{z}_4 \\ i \cdot z_1 & -i \cdot z_2 & z_3 & z_4 & 0 \end{bmatrix} \tag{2.5}$$

$$= \det \begin{bmatrix} 0 & 1 & i & 0 & \dots \\ 1 & 0 & -i & 0 & \dots \\ -i & i & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \bar{z}_3 + \bar{z}_4 \\ \dots & \dots & \dots & z_3 + z_4 & 0 \end{bmatrix}$$

$$= -|z_3 + z_4|^2 \det \begin{bmatrix} 0 & 1 & i \\ 1 & 0 & -i \\ -i & i & 0 \end{bmatrix} = 2|z_3 + z_4|^2, \tag{2.6}$$

where $z_j \in \{0, \pm 1, \pm i\}$ ($j \in [4]$), $z_1 \neq i$, $z_2 \neq -i$ and $z_3, z_4 \neq -1$. Since a positive determinant implies an even (and thus larger than 1) number of negative eigenvalues, it follows that $z_3 + z_4 = 0$. Note that the proof of Proposition 2.16 gives us all possible solutions for $\begin{bmatrix} z_1 & z_2 & z_3 \end{bmatrix}$. We remove those with $z_3 = 1$, since $z_4 = -1$ is not allowed. Besides $z = 0$, we obtain $z = \begin{bmatrix} 1 & 1 & 0 & 0 \end{bmatrix}$, $\begin{bmatrix} -1 & -1 & 0 & 0 \end{bmatrix}$, $\begin{bmatrix} -i & 0 & -i & i \end{bmatrix}$,

$\begin{bmatrix}0 & i & i & -i\end{bmatrix}$. The solution $z = 0$ makes the fifth vertex an isolated vertex, whereas each of the other solutions makes it a twin of one of the four other vertices.

The proof for $D[U] \cong T_b^-$ is analogous to the above and therefore omitted. □

Using Lemma 2.18, we are able to extend its claim to arbitrarily large n.

Lemma 2.19. *Suppose that D is a digraph of order $n > 5$, that contains T_a^-, T_b^- or K^-. Moreover, suppose that D has exactly one negative eigenvalue. Then D is not reduced.*

Proof. By contradiction. Suppose that D is reduced and let $U \subset V(D)$ be such that $D[U]$ is either K^-, T_a^- or T_b^-. Fix some $u' \in V(D) \setminus U$ such that $U^* = U \cup \{u'\}$ induces a weakly connected subdigraph $D[U^*]$. By Lemma 2.18, there is a vertex in U, say u, such that u and u' are twins in $D[U^*]$. If we let $U' = U^* \setminus \{u\}$, then $D[U] \cong D[U']$.

Because D is assumed to be reduced, there is some vertex $w \in V(D) \setminus U^*$ that distinguishes u from u'. Let $W = U \cup \{w\}$ and $W' = U' \cup \{w\}$ and observe that, by Lemma 2.18, w is twin to a member of U and U' in $D[W]$ and $D[W']$, respectively. Now, let v be a vertex in $U \setminus \{u\}$ with valency 3 in $D[U]$. Note that regardless of the choice of u, such a vertex exists for each of the cases for $D[U]$. Moreover, the relation to v (in-neighbor, out-neighbor, undirected neighbor or no neighbor) is different for each of the four vertices in $D[U]$. This implies that the relation of w to v determines which of the vertices in U is the twin of w in $D[W]$.

Suppose that the twin of w in $D[W]$ is u. Then the twin of w in $D[W']$ is u', because u and u' have the same relation to v. But then w does not distinguish u from u', since it is not adjacent to either of the two. This means that the twin of w in $D[W]$ must be a member of $U \setminus \{u\} = U' \setminus \{u'\}$. Specifically, it is the same vertex as the twin of w in $D[W']$, as a consequence of the unique relation to v. But this twin does not distinguish u from u' (as $D[U] \cong D[U']$), so neither does w, and we have our final contradiction. Thus, D is not reduced. □

By Lemmas 2.17 through 2.19, we now have all the necessary tools to prove Theorem 2.14.

Proof. (Of Theorem 2.14.) Suppose D is a reduced digraph of order n with rank larger than 2 and exactly one negative eigenvalue. Since any digraph of order at most 2 has rank at most 2, it follows that $n \geq 3$. Next, we distinguish two cases: either D contains at least one of T_a^-, T_b^-, K^- or it does not. In the former case, we have by

Lemmas 2.18 and 2.19 that $n \leq 4$, otherwise we would lose the reducedness of D. In the latter case, the same conclusion follows unless $n \leq 3$, by Lemma 2.17.

We are thus left with two possibilities: either $n = 3$ or $n = 4$. If $n = 3$, we have that $D = T^-$, by Corollary 2.15.1. Finally, if $n = 4$, then by Proposition 2.16 it holds that $D \in \{T_a^-, T_b^-, K^-\}$. □

We are, in fact, able to conclude much more. Using that the numbers of positive and negative eigenvalues do not change when twin reduction is applied, the results of Theorem 2.14 extend to the underlying structure of any digraph with a single negative eigenvalue. This key observation is formalized in Theorem 2.20.

Theorem 2.20. *Let D be a digraph of order $n \geq 5$, rank larger than 2, with exactly one negative eigenvalue. Then one of the following cases is true.*

(i) Rank$(D) = 3$ and either $TR(D) = T^-$, $TR(D) = T_a^-$ or $TR(D) = T_b^-$,

(ii) Rank$(D) = 4$ and $TR(D) = K^-$.

Proof. Let $D' = TR(D)$. Then D' is reduced and has exactly one negative eigenvalue, which by Theorem 2.14 implies that $D' \in \{T^-, T_a^-, T_b^-, K^-\}$. The claim clearly follows. □

In particular, we observe that if one is given a spectrum that contains three positive, one negative, and arbitrarily many zero eigenvalues, one could say with certainty that the underying structure of the corresponding digraph is exactly K^-. In other words, this digraph is a twin expansion of K^-. Inspired by this fact, the author was convinced that many SHDS digraphs were within reach. Consider, for example, a spectrum of the form

$$\Sigma = \left\{t_1^{[3]}, 0^{[4t_1+t_0-4]}, -3t_1\right\} \text{ for } t_1 \in \mathbb{N}, t_0 \in \mathbb{N}_0.$$

It is now not hard to show that this spectrum belongs to D, obtained from K^- as $D = TE\left(K^-, \begin{bmatrix} t_0 & t_1 & t_1 & t_1 & t_1 \end{bmatrix}\right)$ by considering $\sum_{\mu\in\Sigma} \mu^2$, $\sum_{\mu\in\Sigma} \mu^3$ and Theorem 2.20. In the next section, we show a more general result, based on these principles.

As mentioned before, any rank 2 digraph trivially has precisely one negative eigenvalue. For completeness, we recall that a digraph has rank 2 if and only if $\Gamma(TR(D))$ is either K_2, P_3, or K_3, where in the latter case it must additionally be required that

$TR(D)$ contains an odd number of arcs. For more detail, the interested reader is referred to the full characterization in [83].

2.5 An infinite family of connected SHDS digraphs

We have so far restricted ourselves to *reduced* digraphs, as digraphs that admit to this assumption are in a sense the fundamental structure to the digraphs that may be obtained by introducing twin vertices. In this section, we will be relaxing said assumption and consider twin expansions of the digraphs from Theorem 2.14, to further inquire into the class of digraphs with exactly one negative eigenvalue. In particular, we use that there is exactly one of those digraphs with rank four, to arrive at a remarkable conclusion.

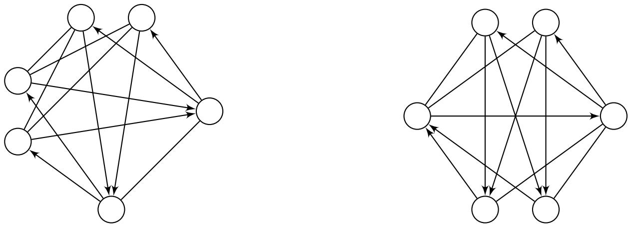
The main result of this section is Theorem 2.23, in which we show that any digraph $D = TE(K^{-}, t)$, where $t = \begin{bmatrix} t_0 & t_1 & t_1 & t_1 & t_2 \end{bmatrix}$ is an expansion vector, is strongly determined by its Hermitian spectrum. In other words, we obtain an infinite family of digraphs that is SHDS, which includes the first such connected infinite family.

As was briefly touched on in the introduction, such digraphs are incredibly rare, as there is an extreme degree of similarity within the collection of Hermitian adjacency matrices of a given order, informally speaking. Even when one just considers a digraph and its converse, which are clearly cospectral but in general not isomorphic, and hence in general not SHDS. Indeed, one is easily convinced that any SHDS digraph is necessarily *self-converse*, which is by itself an extremely rare property. Indeed, by evaluation of the counting polynomials by Harary [59] and Harary and Palmer [60], one is easily convinced that the claim "the fraction of self-converse digraphs of order n goes to zero as n goes to infinity" should be true. This idea is confirmed in Chapter 3.

First, we observe that, regretfully, there are still many twin expansions of K^{-} that we may not determine uniquely from their spectra, as the following example illustrates.

Example 2.3. *Let* $t = \begin{bmatrix} 0 & 2 & 2 & 1 & 1 \end{bmatrix}$ *and* $t' = \begin{bmatrix} 0 & 2 & 1 & 2 & 1 \end{bmatrix}$. *Then* $D = TE(K^{-}, t)$ *and* $D' = TE(K^{-}, t')$ *are* H*-cospectral by Lemma 2.10. However, they are clearly not isomorphic, as is visible in Figure 2.7:* D *contains* 5 *digons, whereas* D' *contains only* 4.

Example 2.3 clearly illustrates the main obstacle in this part of our quest to construct SHDS digraphs; expansion vectors that are closely related, but which do not



(a) D **(b)** D'

Figure 2.7 – Digraphs illustrated in Example 2.3.

quite yield isomorphic digraphs when used to expand K^-. Specifically, permutations of the same expansion vector yield cospectral, but not necessarily isomorphic, digraphs. This observation is formalized in the following lemmas.

Lemma 2.21. *Let $t_0 \in \mathbb{N}_0$, $\tau \in \mathbb{N}^4$ and let τ' be a permutation of τ. If $t = \begin{bmatrix} t_0 & \tau \end{bmatrix}$ and $t' = \begin{bmatrix} t_0 & \tau' \end{bmatrix}$, then $TE(K^-, t)$ and $TE(K^-, t')$ are cospectral.*

Proof. Immediate from Lemma 2.10. □

Lemma 2.22. *Let $t_0 \in \mathbb{N}_0$ and let $\tau \in \mathbb{N}^4$ be such that fewer than three entries of τ are equal. Then there exists a $\tau' \neq \tau$, obtained as a permutation of τ, such that if $t = \begin{bmatrix} t_0 & \tau \end{bmatrix}$ and $t' = \begin{bmatrix} t_0 & \tau' \end{bmatrix}$, then $TE(K^-, t) \ncong TE(K^-, t')$.*

Proof. By contradiction. Recall that $(1, 2)$ and $(3, 4)$ are digons in K^-, and that two digraphs may only be isomorphic if they contain equal numbers of digons. Let $t = \begin{bmatrix} t_0 & t_1 & t_2 & t_3 & t_4 \end{bmatrix}$, and assume that no three t_j's are equal. ($j = 1, \ldots, 4$.) Let $t' = \begin{bmatrix} t_0 & t_1 & t_3 & t_2 & t_4 \end{bmatrix}$ and $t'' = \begin{bmatrix} t_0 & t_1 & t_4 & t_3 & t_2 \end{bmatrix}$. Suppose that all three t construct isomorphic expansions. Then by counting digons

$$\begin{cases} TE(K^-, t) \cong TE(K^-, t') \\ TE(K^-, t) \cong TE(K^-, t'') \end{cases} \implies \begin{cases} t_1t_2 + t_3t_4 = t_1t_3 + t_2t_4 \\ t_1t_2 + t_3t_4 = t_1t_4 + t_2t_3 \end{cases}$$
$$\implies \begin{cases} (t_1 - t_4)(t_2 - t_3) = 0 \\ (t_1 - t_3)(t_2 - t_4) = 0 \end{cases}$$

and thus $t_1 = t_2 = t_3$, $t_1 = t_2 = t_4$, $t_1 = t_3 = t_4$, or $t_2 = t_3 = t_4$, which is a contradiction. □

From Lemma 2.22, we find the following necessary condition for SHDS expansions of K^-.

Corollary 2.22.1. *$D = TE\left(K^-, \begin{bmatrix} t_0 & \tau \end{bmatrix}\right)$, $t_0 \in \mathbb{N}_0$, $\tau \in \mathbb{N}^4$, is SHDS only if at least three entries of τ are equal.*

Intuitively, one might also say that if the condition in Corollary 2.22.1 is satisfied, then any permutation of t would yield digraphs that are isomorphic to one another. In other words, that the condition above is not just necessary, but also sufficient. In the theorem below, which the author considers to be the main contribution of this paper, we show exactly that.

Theorem 2.23. *Let t be an expansion vector. Then $D = TE(K^-, t)$ is SHDS if and only if $t = \begin{bmatrix} t_0 & \tau \end{bmatrix}$, where $t_0 \in \mathbb{N}_0$ and τ is a permutation of $\begin{bmatrix} t_1 & t_1 & t_1 & t_2 \end{bmatrix}$, $t_1, t_2 \in \mathbb{N}$.*

Proof. Necessity was addressed in Corollary 2.22.1, so we will only show sufficiency. Let D^* be a digraph and suppose that $\Sigma_D = \Sigma_{D^*}$. If we can show $D \cong D^*$, the claim is true. Since D has rank 4 with three positive eigenvalues, we know by Theorem 2.20 that $D^* = TE(K^-, b)$ for some expansion vector $b = \begin{bmatrix} b_0 & b_1 & b_2 & b_3 & b_4 \end{bmatrix}$. Moreover, by Corollary 2.10.1, D^* has eigenvalue t_1 with multiplicity 2. Since $t_1 > 0$, the eigenvectors corresponding to eigenvalue t_1 are orthogonal to the nullspace of $H = H(D^*)$. Therefore, the eigenvalues are constant on the four nontrivial parts of D^* and 0 on the isolated vertices in D^*. That is, the eigenvectors z corresponding to t_1 satisfy

$$z = \begin{bmatrix} \mathbf{0} & z_1\mathbf{j_1} & z_2\mathbf{j_2} & z_3\mathbf{j_3} & z_4\mathbf{j_4} \end{bmatrix}^\top \quad \text{for} \quad z_1, z_2, z_3, z_4 \in \mathbb{C}. \tag{2.7}$$

Recall that Hermitian matrices are diagonalizable [11] and that diagonalizable matrices have geometric multiplicities equal to their algebraic multiplicities. Hence, there are two independent eigenvectors z and w that correspond to t_1 and satisfy (2.7). Moreover, any linear combination of z and w is again an eigenvector for t_1. Hence, there is an eigenvector x that is obtained as such a linear combination, which is zero for any one of the nontrivial parts of D^*. Suppose that at least one of x_2, x_3, x_4 is nonzero and

$$x = \begin{bmatrix} \mathbf{0} & \mathbf{0} & x_2\mathbf{j_2} & x_3\mathbf{j_3} & x_4\mathbf{j_4} \end{bmatrix}^\top \quad \text{and} \quad Hx = t_1 x, \tag{2.8}$$

where

$$H = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & J & iJ & -iJ \\ 0 & J & 0 & -iJ & iJ \\ 0 & -iJ & iJ & 0 & J \\ 0 & iJ & -iJ & J & 0 \end{bmatrix}$$

for blocks H_{ij} of appropriate dimensions. Working out the latter equality in (2.8), we obtain

$$\begin{cases} b_2x_2 + ib_3x_3 - ib_4x_4 = 0 \\ -ib_3x_3 + ib_4x_4 = t_1x_2 \\ ib_2x_2 + x_4 = t_1x_3 \\ -ib_2x_2 + b_3x_3 = t_1x_4 \end{cases}$$

from which it follows that $b_2x_2 = t_1x_2$, $b_3x_3 = t_1x_3$ and $b_4x_4 = t_1x_4$. Moreover, at most one of x_2, x_3, x_4 can be zero and therefore at least two of b_2, b_3, b_4 are equal to t_1. But similarly, this implies that at least two among each three of b_1, b_2, b_3, b_4 equals t_1, and thus at least three of b_1, b_2, b_3, b_4 are equal to t_1. Thus, since the last four numbers may be permuted to any order without changing the spectrum, we may assume without loss of generality that $b = \begin{bmatrix} b_0 & t_1 & t_1 & t_1 & b_4 \end{bmatrix}$.

Finally, by comparing the number of edges in the underlying graph, we obtain $b_4 = t_2$, and since $|\Sigma_D| = |\Sigma_{D^*}|$, we have $b_0 = t_0$. Hence, if $\Sigma_D = \Sigma_{D^*}$ then $b = t$ and thus $D^* \cong D$. □

Thus, by Theorem 2.23, we may be certain that we may uniquely determine each digraph whose Hermitian spectrum is of the form

$$\left\{-\sqrt{3t_1t_2 + t_1^2} - t_1,\ \sqrt{3t_1t_2 + t_1^2} - t_1,\ t_1^{[2]},\ 0^{[t_0+3t_1+t_2-4]}\right\}, t_0 \in \mathbb{N}_0, t_1, t_2 \in \mathbb{N}.$$

2.6 Closing remarks regarding WHDS digraphs

While most of this chapter has been concerned with strong determination by the Hermitian spectrum, we conclude with some remarks on its weaker counterpart. It stands to reason that the digraphs that are not SHDS due to the problem illustrated in Example 2.3 might be WHDS, as most of the machinery that was used to show Theorem 2.23 is still in place. We first observe that it is in general not true that any expansion of K^- is WHDS, after which we prove an analogue to Proposition 2.3.

As mentioned before, relaxing the connectivity assumption may yield cospectral digraphs with distinct underlying graphs, which implies that said digraphs are not switching equivalent. Recall the following example by Wang et al. [107].

Example 2.4. *[107] Consider the two digraphs D and D^*, obtained from T^- as $D = TE\left(T^-, \begin{bmatrix} t_0 & 3 & 3 & 18 \end{bmatrix}\right)$ and $D^* = TE\left(T^-, \begin{bmatrix} t_0+4 & 2 & 9 & 9 \end{bmatrix}\right)$, for some $t_0 \in \mathbb{N}_0$. Then $\Sigma_D = \Sigma_{D^*}$ (plug in (2.2)) regardless of t_0. Since D and D^* do not contain an equal number of isolated vertices, they cannot be switching equivalent. Thus, there are infinitely many pairs of cospectral mates. Most notably, suppose that $t_0 = 0$. Then D is connected, but not switching equivalent to D^*, while they are cospectral. Thus, D is not WHDS, even when $t_0 = 0$.*

As we have seen throughout this paper, there are many parallels between T^- and K^-. This has caused us to believe that a similar phenomemon occurs for the negative tetrahedron. As we will see shortly, there are indeed pairs of expansion vectors t, t' for K^- such that $D = TE(K^-, t)$ and $D' = TE(K^-, t')$ are both connected and have the same nonzero eigenvalues, but not the same number of vertices, which allows us to formulate an analogue of Proposition 2.4.

Proposition 2.24. *There are infinitely many rank 4 digraphs with exactly one negative eigenvalue that are not WHDS.*

The correctness of Proposition 2.24 follows immediately from the following example.

Example 2.5. *Let $t_0 \in \mathbb{N}_0$ and consider the vectors $t = \begin{bmatrix} t_0 & 9 & 18 & 20 & 60 \end{bmatrix}$ and $t' = \begin{bmatrix} t_0+4 & 10 & 12 & 36 & 45 \end{bmatrix}$. Then $D = TE(K^-, t)$ and $D' = TE(K^-, t')$ both have characteristic polynomial*

$$\chi(\mu) = \mu^{103+t_0}(\mu^4 - 3522\mu^2 + 90720\mu - 583200). \tag{2.9}$$

Moreover, as the two contain distinct numbers of isolated vertices, they are clearly not switching equivalent.

However, it should also be noted that such examples have proven to be extremely rare. If one enumerates all vectors $t = \begin{bmatrix} 0 & t_1 & t_2 & t_3 & t_4 \end{bmatrix}$ with[7] $0 < t_1 \leq t_2 \leq t_3 \leq$

[7] Note that this does not restrict the investigation, as we are not interested in switching equivalent pairs.

$t_4 \leq 104$ and computes the characteristic polynomials corresponding to $TE(K^-, t)$ via Lemma 2.10, we find as few as five characteristic polynomials whose nonzero roots do not occur uniquely. Out of these five polynomials, $\chi(\mu)$ as in (2.9) is of smallest order; the corresponding digraphs contain at least 107 vertices. For the remaining digraphs, we obtain strong evidence that they are WHDS. In particular, we may thus conclude the following.

Proposition 2.25. *Any digraph of order less than* 107 *that has rank* 4 *and exactly one negative eigenvalue is WHDS.*

Proof. It is clear that any pair of digraphs $D = TE(K^-, [0 \;\; \tau])$, $D' = TE(K^-, [0 \;\; \tau'])$ with $|V(D)|, |V(D')| < 107$ and equal nonzero eigenvalues would have occurred in the performed enumeration. Since they did not, and the number of isolated vertices that may be added is bounded by the assumption on the order of the digraphs, the claim follows. $\square$

Proposition 2.26. *Let* $t_0 \in \mathbb{N}_0, \tau \in \mathbb{N}$ *with* $\tau_j \leq 7$, $j = 1, \ldots, 4$. *Then* $TE(K^-, [t_0 \;\; \tau])$ *is WHDS.*

Proof. Let $t = [t_0 \;\; \tau]$ with $\tau_j \leq 7$, $j \in [4]$, and $t' = [t_0 \;\; \tau']$ where τ' contains at least one element larger than 100. Then

$$\sum_{1 \leq i < j \leq 4} t_i t_j \leq 294 < 306 \leq \sum_{1 \leq i < j \leq 4} t'_i t'_j.$$

Thus, if there were expansion vectors that would have yielded the same characteristic polynomial coefficients as t, they would have occurred in the performed enumeration. $\square$

Moreover, if we assume connectivity, we obtain a result similar to Proposition 2.3.

Proposition 2.27. *Any two connected, cospectral rank* 4 *digraphs with exactly one negative eigenvalue are switching equivalent.*

Proof. Let D_1 and D_2 be connected, cospectral, rank 4 digraphs with exactly one negative eigenvalue. By Theorem 2.20, $TR(D_1) = TR(D_2) = K^-$. Let t, s be such that $D_1 = TE(K^-, t)$ and $D_2 = TE(K^-, s)$. (Note that $t_0 = s_0 = 0$ is implied.)

We first observe that s may be obtained as a permutation of t. Indeed, consider equations (2.10)-(2.13), which should all hold simultaneously by Lemma 2.10. (Note that (2.10) is implied by $t_0 = s_0$.) Then, if these elementary symmetric polynomials in $\{t_1, t_2, t_3, t_4\}$ and $\{s_1, s_2, s_3, s_4\}$ are the same, s is indeed distinct from t by at most a reordering of its entries.

$$\sum_{j=1}^{4} t_j = \sum_{j=1}^{4} s_j \tag{2.10}$$

$$\sum_{1 \leq i < j \leq 4} t_i t_j = \sum_{1 \leq i < j \leq 4} s_i s_j \tag{2.11}$$

$$\sum_{1 \leq i < j < k \leq 4} t_i t_j t_k = \sum_{1 \leq i < j < k \leq 4} s_i s_j s_k \tag{2.12}$$

$$\prod_{j=1}^{4} t_j = \prod_{j=1}^{4} s_j \tag{2.13}$$

Now, observe that any permutation of t might be obtained by a sequence of pairwise interchanges of elements. Thus, if we can show that every such pairwise exchange yields a switching equivalent digraph, we are done. Suppose that t' is obtained from t by interchanging elements t_u and t_v, $u, v \in [4]$, and let $D = TE(K^-, t)$ and $D' = TE(K^-, t')$. We distinguish two cases: either (u, v) is a digon in K^- or it is not. Note that we may assume without loss of generality that $(u, v) = (1, 2)$ in the former case, and $(u, v) = (1, 3)$ in the latter.

Suppose that $(u, v) = (1, 2)$. Then $D' \cong D^c$, and thus D is switching equivalent to D'. Finally, suppose that $(u, v) = (1, 3)$ and let $S = \mathrm{Diag}\left(\begin{bmatrix} -i \cdot \mathbf{j}_{t_1} & \mathbf{j}_{t_2} & i \cdot \mathbf{j}_{t_3} & \mathbf{j}_{t_4} \end{bmatrix}\right)$. If we let D_S be the digraph determined by the Hermitian $H_S = S^{-1} H(D) S$, then $D_S \cong D'$. Since D_S was obtained from D by a four-way switching, D is again switching equivalent to D', which completes the proof. $\square$

CHAPTER 3

Self-converse digraphs are extremely rare

Abstract

A digraph is cospectral to its converse, with respect to the usual adjacency matrices. Hence, it is easy to see that a digraph whose eigenvalues occur uniquely, up to isomorphism, must be isomorphic to its converse. It is therefore natural to ask whether or not this is a common phenomenon. This note contains the theoretical evidence to confirm that the fraction of self-converse digraph tends to zero.

3.1 Introduction

With the rising interest in spectral characterization of digraphs and some of their generalizations came an interesting question, concerning the existence of a fairly obvious pairs of cospectral digraphs. At the heart of this issue is the fact that a digraph and its converse, obtained from the former by reversing all of the oriented edges, are typically encoded by matrices that are each other's conjugate transpose. In other words, two digraphs that may not be equivalent, are almost trivially cospectral. Thus, in order for a digraph to be determined by its spectrum in the traditional way [27], it must be isomorphic to its converse; such digraphs are said to be *self-converse* [9].

This then raises the following question: *how rare are self-converse digraphs?* In Chapter 2, numerical evidence (see Table 3.1, below) suggesting that the fraction of self-converse digraphs converges to zero as the number of vertices n goes to infinity was provided, although a formal proof to this claim has not appeared yet. Specifically, while the counting polynomials by [60, 59] are quite easily evaluated, they are relatively unwieldy objects to work with, for arbitrary n. In this note, we will present a simple proof, to formally show the desired result.

3.2 Main result

The discussion in this chapter essentially involves the existence of a non-trivial automorphism in a random graph. See Section 1.1 of automorphism, and recall the Erdős-Rényi random graph $\Gamma(n,p)$, and its natural directed analog $D(n,p)$. $\Gamma(n,p)$ is the order-n graph such that every edge occurs with probability p. That is, $\mathbb{P}(\{u,v\} \in E) = p$. Accordingly, $D(n,p)$ is the order-n digraph whose arcs uv occur with probability p; if both arcs uv and vu occur, we say instead that the edge $\{u,v\}$ occurs.

The key argument used in the proof of the main result is the notion that almost all symmetric subgraphs of a random directed graph $D(n,1/2)$ have no nontrivial automorphism. For completeness, a proof of this essentially well-known fact for the desired Erdős-Rényi graph $\Gamma(n,p=1/4)$ is included, below.

Key to the discussion below is the idea that the existence of edges in a random graph with some probability p corresponds to a Bernoulli trial. These are well-known to exhibit *concentration around the mean*, which is formalized (among others) by the so-called Chernoff bounds.

Theorem 3.1 (Chernoff bounds [20])**.** *Let X_j be n independent Bernoulli variables,* *let* $X = \sum_j^n X_j$, *and let* $\mu = \mathbb{E}(X)$. *Then, we have:*

$$\mathbb{P}[X \geq (1+\delta)\mu] \leq \exp\left(\frac{-\delta^2\mu}{2+\delta}\right) \quad (\delta > 0), \quad \textit{and} \tag{3.1}$$

$$\mathbb{P}[X \leq (1-\delta)\mu] \leq \exp\left(\frac{-\delta^2\mu}{2}\right) \quad (0 < \delta < 1). \tag{3.2}$$

By a straightforward application of the above, one may then draw asymptotic conclusions regarding the number of neighbors of a vertex, and common neighbors of a pair of vertices.

Lemma 3.2. *Let* $\Gamma = \Gamma(n, 1/4)$ *and* $\epsilon > 0$ *be arbitrarily small. The vertices of* Γ *have degree at least* $\frac{n}{4}(1-\epsilon)$ *and at most* $\frac{n}{8}(1+\epsilon)$ *common neighbors, with high probability (as* n *goes to infinity).*

Now, the following is an easy adaptation from [86, Thm. 3.1].

Theorem 3.3 ([86])**.** *With high probability, the random graph* $\Gamma(n, p = 1/4)$ *is asymmetric (as* n *goes to infinity).*

Proof. Let $V = \{1, 2, \ldots, n\}$ be the vertex set of $\Gamma = \Gamma(n, 1/4)$ and let $f : V \mapsto V$ be an automorphism such that $f(x) = y$ for some vertices $x \neq y$. Let $M = \{v \in V : f(v) \neq v\}$ be the set of vertices that are moved by f. Moreover, let $V' = \binom{V}{2}$, and let $f' : V' \mapsto V'$ be the permutation defined by $f'(\{u, v\}) = \{f(u), f(v)\}$.

By Lemma 3.2, for sufficiently large n, there exist at least $\lceil \frac{n}{4}(1-\epsilon) - \frac{n}{8}(1+\epsilon)\rceil = \lceil \frac{n}{8}(1-3\epsilon)\rceil$ vertices that are connected by an edge to x but not to y. All of these vertices are moved by the automorphism f. Therefore, $|M| \geq cn$ for $c = (1-3\epsilon)/8$ with ϵ small. Thus the number of pairs of vertices that are moved by this automorphism is at least $\binom{cn}{2} - n \geq c'n^2$ for

$$c' = \frac{c^2 n - c}{2n} \xrightarrow[n\to\infty]{} \frac{1 - 6\epsilon + 9\epsilon^2}{128} > 0 \text{ for } \epsilon \neq \frac{1}{3}$$

and sufficiently large n. Therefore, the number of cycles of f' is at most $k = \binom{n}{2} - c'n^2/2$.

If f is an automorphism of Γ, then the pairs in one cycle of f' are either all edges or they are all non-edges of Γ. Hence, there are at most 2^k graphs such that f is their automorphism.

Combining the above, it follows that the probability that $\Gamma(n, 1/4)$ has a non-identity automorphism is at most

$$\frac{n! \cdot 2^{\binom{n}{2} - c'n^2/2}}{2^{\binom{n}{2}}} \leq \frac{n^n}{2^{c'n^2/2}},$$

which tends to 0 as $n \to \infty$. Indeed, note that

$$\log\left(\frac{n^n}{2^{c'n^2/2}}\right) = n \log n - \frac{1}{2}c'n^2 \log 2 \xrightarrow[n\to\infty]{} -\infty,$$

for all $c' > 0$. □

In fact, Erdős and Rényi [33] have shown that Theorem 3.3 holds whenever $\min\{p, 1-p\} \leq (1-\epsilon)n \log n$. Here, $n \log n$ is the so-called *threshold value*; see [39] for more detail.

The next result now follows naturally, by observing that any relabeling of the vertices that maps a digraph D to D^c simultaneously maps its symmetric subgraph onto itself. Indeed, since the latter implies with high probability that said mapping is, in fact, the identity mapping, a contradiction follows.

Proposition 3.4. *The probability that $D(n, 1/2)$ is self-converse tends to zero as $n \to \infty$.*

Proof. Let $n \to \infty$, and let D be an order-n digraph graph whose symmetric subgraph is G. If $D = D(n, 1/2)$, then G is the order-n Erdős-Rényi graph with edge probability $\frac{1}{4}$. By Theorem 3.3, G has no nontrivial automorphism with high probability. Now, since any isomorphism from D to D^c is an automorphism of G, said isomorphism must be the identity map. However, with high probability, there is a pair $(x, y) \in V \times V$ such that $E(D)$ contains the arc (x, y) but not its converse arc (y, x). Therefore, the identity map is no isomorphism from D to D^c (with high probability), thus yielding a contradiction. □

One should be somewhat mindful of what is being counted. Proposition 3.4 implies that the fraction of self-converse *labeled* digraphs tends to zero, whereas we are interested in its unlabeled counterpart, i.e., the fraction of all non-isomorphic digraphs. Note the significant distinction: any digraph with only the identity automorphism has $n!$ labeled versions, whereas (e.g.) the complete graph only has one. In other words, the former is weighted much more heavily than the latter, by a probabilistic argument. Fortunately, this does not invalidate the approach. In their extensive book, Harary and Palmer [61] prove that almost all graphs of order n can be labeled in $n!$ ways, and observe:

Theorem 3.5 ([61])**.** *Most labeled graphs have property "P" if and only most unlabeled graphs have property "P".*

It should be clear that the argumentation would directly carry over to digraphs. Hence, the desired result follows from Proposition 3.4.

Proposition 3.6. *The fraction of order-n self-converse digraphs tends to zero as* $n \to \infty$.

3.3 Convergence rate

To give some idea as to the rate at which the fraction of self-converse digraphs tends to zero, we include Table 3.1, below. Here, $f(n)$ denotes said fraction of the non-isomorphic digraph of order n, obtained by evaluation of counting polynomials from [60, 59].

n	3	4	5	6	7	8
$f(n)$	$6.25{\cdot}10^{-1}$	$3.21{\cdot}10^{-1}$	$7.36{\cdot}10^{-2}$	$9.87{\cdot}10^{-3}$	$6.16{\cdot}10^{-4}$	$2.20{\cdot}10^{-5}$
n	9	10	11	12	13	14
$f(n)$	$3.89{\cdot}10^{-7}$	$3.79{\cdot}10^{-9}$	$1.85{\cdot}10^{-11}$	$4.89{\cdot}10^{-14}$	$6.50{\cdot}10^{-17}$	$4.58{\cdot}10^{-20}$
n	15	16	17	18	19	20
$f(n)$	$1.63{\cdot}10^{-23}$	$3.06{\cdot}10^{-27}$	$2.90{\cdot}10^{-31}$	$1.43{\cdot}10^{-35}$	$3.59{\cdot}10^{-40}$	$4.64{\cdot}10^{-45}$

Table 3.1 – The fraction $f(n)$ of digraphs of order n that is self-converse.

CHAPTER 4

Spectral properties of signed directed graphs

Abstract

The spectral properties of signed directed graphs, which may be naturally obtained by assigning a sign to each edge of a directed graph, have received substantially less attention than those of their undirected and/or unsigned counterparts. To represent such signed directed graphs, we use a striking equivalence to $\mathbb{T}_6$-gain graphs to formulate a Hermitian adjacency matrix, whose entries are the unit Eisenstein integers $\exp(k\pi i/3)$, $k \in \mathbb{Z}_6$. Many well-known results, such as (gain) switching and eigenvalue interlacing, naturally carry over to this paradigm. We show that non-empty signed directed graphs whose spectra occur uniquely, up to isomorphism, do not exist, but we provide several infinite families whose spectra occur uniquely up to switching equivalence. Intermediate results include a classification of all signed digraphs with rank $2, 3$, and a deep discussion of signed digraphs with extremely few (1 or 2) non-negative (eq. non-positive) eigenvalues.

4.1 Introduction

While the spectral perspective on complex unit gain graphs is still relatively fresh, various special cases have been studied to a varying extent. Most prominently, signed graphs [109, 5], which may effectively be thought of as ‘real unit gain graphs,’ have received considerable attention. Moreover, the Hermitian adjacency matrices H and N for mixed graphs [51, 76, 84] also come to mind. These have, in hindsight, simply allowed subsets of $\mathbb{T}$ and accompanied the relevant entries with an appropriate interpretation to represent directed graphs.

Most relevantly, in [84], the allowed entries are $\{\exp(ik\pi/3) \mid k \in \{-1, 0, 1\}\}$, where the strictly real entry represents a digon, and those with a nonzero imaginary part represent arcs. This chapter generalizes that line, allowing gains in the subgroup $\{\exp(ik\pi/3) \mid k \in [6]\} =: \mathbb{T}_6$. Accordingly, the corresponding matrices naturally represent *signed directed graphs*.

Albeit quietly, these objects are often useful in the modeling of dynamical systems, such as classical predator-prey populations [105]. In this context, a dedicated group of researchers (see, e.g., [16, 57, 105]) has been studying signed digraphs stemming from *sign-pattern matrices*; effectively imposing no assumptions on the conversion rate between states in such a system, other than the sign of the effect. Conclusions regarding, e.g., the stability of a (or, sometimes, any) system with the corresponding signs are obtained using spectral techniques. In contrast, this chapter focuses on the above-mentioned gain graph representation of a signed directed graph, and the spectral consequences thereof.

Our ultimate interest lies with the question whether or not this representation of signed directed graphs may offer sufficient combinatorial information, in order to uniquely determine such a signed directed graph, when given its spectrum. The answer to this question consists of two parts. First, we show that any signed directed graph has a partner that is switching equivalent (and thus cospectral), but not isomorphic. This is a natural consequence of the fact that $\mathbb{T}_6$ is closed under multiplication, due to which it is always possible to apply gain switching and obtain a non-isomorphic signed directed graph. We do, however, obtain several families of signed directed graphs that are switching equivalent to every signed directed graph to which they are cospectral.

In order to streamline the discussion, we first set out to classify signed directed graphs that satisfy particular spectral conditions. We show that one may without loss of generality assume the gains of a spanning tree, which aids the classification significantly. By applying this idea, in conjunction with eigenvalue interlacing we classify all signed directed graphs whose rank is 2 or 3; we find a notably concise characterization of all such signed digraphs, which may be described as twin expansions of either an edge, a triangle, or the transitive tournament of order four.

Subsequently, we provide an extensive discussion of signed directed graphs with exactly 1 or 2 non-negative eigenvalues. We show that such graphs are highly dense and provide a list of necessary properties, though already in the case of 2 non-negative eigenvalues, the complete list of candidates quickly becomes unwieldy. Thus, we focus on a few special cases, such as clique expansions of the 5-cycle and the 4-path. In particular, we characterize all signed directed graphs on these minimally dense graphs, such that the resulting signed digraphs admit to the imposed requirements.

The above characterizations are then used to consider spectral determination. Through a series of counterexamples, we show that the discussed low rank signed digraphs are not, in general, determined by their spectra. However, by applying a sequence of counting arguments to the lists obtained above, we are then able to prove that, among others, several of the families with 2 non-negative eigenvalues are determined by their spectrum. Specifically, in addition to a number of sporadic examples, we find several arbitrarily large graphs, obtained as clique expansions of C_4, P_4 or C_5, that admit signed digraphs cospectral only to switching equivalent signed digraphs.

The contents of this chapter are organized as follows. We first provide a thorough introduction of the subject matter, in Section 4.2. Sections 4.3 and 4.4 are concerned with the characterization of signed digraphs that satisfy an imposed set of spectral requirements. The obtained knowledge is then applied in Section 4.5, to investigate spectral characterizations of signed digraphs. Finally, we conclude with a collection of open questions.

The main tools used throughout are eigenvalue interlacing and expansion of graphs via lexicographic products with either empty or complete graphs. Additionally, Lemmas 4.1 and 4.2, which count respectively edges and triangles, and Proposition 4.4, which allows us to fix the signature of a subset of the edges without loss of generality, are frequently applied throughout.

4.2 Preliminaries

The objects studied in this chapter are, in essence, $\mathbb{T}_6$-gain graphs. These are *complex unit gain graphs* [91] whose gain groups are restricted to the multiplicative group

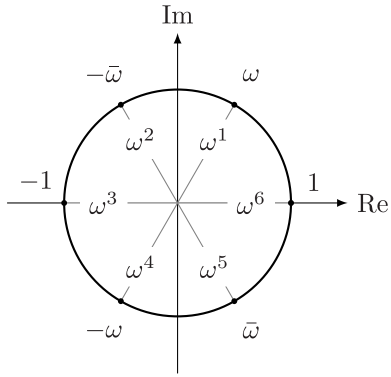


Figure 4.1 – The possible entries of $\mathcal{E}$.

$\mathbb{T}_6 = \{\exp(ik\pi/3) \mid k \in [6]\} = \{\omega^k \mid k \in [6]\}$, and recall that $\omega = (1 + i\sqrt{3})/2$ as is denoted throughout. For further details regarding the terminology and notation, the reader is referred to Section 1.1.

The main discussion in this chapter is concerned with the matrices that are associated with the described structures. The nonzero entries of the so-called Eisenstein matrix $\mathcal{E}(\Phi)$, as defined in Definition 1.3, are exactly the unit elements of the imaginary quadratic ring $\mathbb{Z}[\omega]$. The elements of the latter group are called the Eisenstein integers [45], which justifies the terminology.

As noted before, an Eisenstein matrix whose entries have non-negative real parts coincides exactly with the alternative Hermitian adjacency matrix for directed graphs, proposed by Mohar [84]. Since the negative counterpart to every such (non-zero) entry is also contained in $\mathbb{T}_6$, an arbitrary Eisenstein matrix naturally represents a *signed directed graph*. That is, any $\mathbb{T}_6$-gain graph coincides with the natural Hermitian adjacency matrix[1] of a directed graph whose edges are accompanied with a weight that is either 1 or -1, and vice versa. Hereafter, we will use the latter perspective in our discussion, though the implications and applicable theory of the gain graph equivalent are widely applied.

In the context of signed digraphs, note that the gain $\varphi(C)$ of a cycle C always satisfies $\varphi(C) \in \mathbb{T}_6$. It is sometimes called *real* if $\mathrm{Im}\,(\varphi(C)) = 0$, and it is called *positive* (resp. *negative*) if $\mathrm{Re}\,(\varphi(C)) > 0$ (resp. < 0). Finally, since the real part contains all of the information that is interesting from a spectral point of view (see

[1] Note that the original Hermitian adjacency matrix [51, 76] does not allow for a natural inclusion of the signs, whereas the variant [84] does.

Theorem 1.3), the choice of direction in which a cycles is traversed is, for the purposes of this chapter, inconsequential and thus not specifically mentioned.

4.2.1 Expansions

Similarly to Chapter 2, Sections 4.3 and 4.4 will be looking to construct arbitrarily large signed digraphs, based on smaller structures that we know admit to some predetermined set of requirements. Depending on the context, we will be looking to add either *twins* or *pseudotwins* to a signed digraph. While these conceptual ideas are widely known, we include a formal definition, as the details tend to vary.

In essence, two nodes u and v are twins or pseudotwins if their respective relations to the remaining vertices in V are equivalent. The former additionally requires u and v to be non-adjacent, while the latter requires that they are adjacent and additionally that all triangles containing both u and v have gain 1. Accordingly, twins, twin expansion and twin reduction follow Definitions 2.3 and 2.7, up to the notable absence of isolated vertices for the remainder of this chapter[2]. Further, pseudotwins are defined as follows.

Definition 4.1. *Let $\Phi = (G, \varphi)$ be a signed digraph of order n, whose Eisenstein matrix is $\mathcal{E}$, and let $u, v \in V(\Phi)$ be distinct vertices. If, for some gain switching matrix X and all $z \in V$ we have $(\mathcal{E} + I)_{uz} = (X\mathcal{E}X^{-1} + I)_{vz}$, then u and v are called (switching) pseudotwins.*

Now, as before, we may straightforwardly define an expansion and a reduction operator that respectively grow and shrink signed digraphs, by introducing and removing pseudotwins.

Definition 4.2. *Let $\Phi = (G, \varphi)$ be a signed digraph with an ordered set V of n vertices, and let $\tau \in \mathbb{N}^n$ be an appropriate expansion vector. The clique expansion of Φ with respect to τ is denoted $\Phi' = CE(\Phi, \tau)$ and is obtained by replacing each vertex u in Φ by t_u pseudotwins. Formally, if $V = [n]$, let $V(D') = V_0 \cup V_1 \cup \cdots \cup V_n$, where $V_0, V_1, \ldots, V_n$ are mutually disjoint sets, with $|V_u| = \tau_u$. In Φ', $\mathcal{E}'_{u'v'} = \mathcal{E}_{uv}$ for every $u' \in V_u$, $v' \in V_v$, $u, v \in V$, where $\mathcal{E}$ and $\mathcal{E}'$ are the Eisenstein matrices of Φ and Φ', respectively. Finally, $\mathcal{E}'_{u'v'} = 1$ for every pair of $u', v' \in V_j$, $j \in [n]$*

Alternatively, one may think of the twin expansion and clique expansion operators as taking the lexicographic product (see, e.g., [43]) of a signed digraph Φ with the

[2] Rather than writing the corresponding expansion vectors as $[t_0 = 0 \;\; t_1 \;\; \cdots \;\; t_n]$, the first entry, which would have corresponded to any isolated vertices, is simply discarded throughout this chapter.

collection $\{O_{\tau_1}, O_{\tau_2}, \ldots, O_{\tau_n}\}$, in the case of twin expansion, or $\{K_{\tau_1}, K_{\tau_1}, \ldots, K_{\tau_1}\}$ in the case of clique expansion. Note that the number of nonzero eigenvalues is unaffected by the twin expansion, and the number of eigenvalue unequal to -1 is not affected by clique expansion.

Other authors (e.g., [83, 87]) have used the concepts above with varying notation; the author prefers the definition in terms of operators, to make the distinction between them clear.

Remark 4.1. *Since, for both expansion operators, vertex j is mapped to a group of τ_j vertices, the ordering of τ and the corresponding labeling of the graph that is to be expanded both matter. Without explicit mention hereafter, we will label the vertices of a path graph such that its edges are $(1,2),(2,3),\ldots,(n-1,n)$, and the vertices of a cycle graph such that its edges are $(1,2),(2,3),\ldots,(n-1,n),(n,1)$, for the remainder of this chapter. Other cases will be explicitly illustrated.*

4.2.2 Counting substructures

A well-known result in spectral graph theory is that the number of closed walks in a graph of a given length are, in a sense, counted by the sum of its eigenvalues, exponentiated to the corresponding length. With respect to $\mathcal{E}$, a direct analogue of this idea holds.

Lemma 4.1. *If Φ is a signed digraph such that $\Gamma(\Phi)$ contains m edges. Then $tr\left(\mathcal{E}(\Phi)^2\right) = 2m$.*

Proof. Let $\mathbf{e_j}$ denote the columns of $\mathcal{E} := \mathcal{E}(\Phi)$. Then $\mathcal{E}^2_{jj} = \mathbf{e}_j^*\mathbf{e}_j = d_j$, where d_j is the degree of node j in $\Gamma(\Phi)$. Hence, we have $\operatorname{tr}(\mathcal{E})^2 = \sum_{j=1}^n d_j = 2m$. □

Note that we may categorize the three-cycles into four categories, based on the real part of their gains. The following then straightforwardly follows.

Lemma 4.2. *Let Φ be a signed digraph, and let $s_{(z)}$ denote the number of triangles t with $Re(\varphi(t)) = z$ that are contained in Φ as induced subdigraphs. Then*

$$tr(\mathcal{E})(\Phi)^3 = 6s_{(1)} + 3s_{(1/2)} - 3s_{(-1/2)} - 6s_{(-1)}.$$

Proof. Let $u \in V(\Phi)$ and let Δ_u be the collection of triangles in $\Gamma(\Phi)$ that contain u. Then, we have

$$(\mathcal{E}^3)_{uu} = \sum_{t\in\Delta_u} \varphi(t) = \sum_{z\in\left\{\pm 1, \pm\frac{1}{2}\right\}} 2z \cdot c_{(z)},$$

where $c_{(z)}$ denotes the number of triangles t with Re $\varphi(t) = z$ in Φ contain u. Here, the second equality holds since every triangle is traversed in two directions. Specifically, recall that the gains of such mirror traversals are each others complex conjugate, and $\alpha + \bar{\alpha} = 2\text{Re } \alpha$ for $\alpha \in \mathbb{C}$. The claim then follows, since every triangle counted thrice: once for every vertex it contains. $\square$

4.2.3 Switching equivalence and isomorphism

In the later parts of this chapter, we will be looking to classify signed digraphs that are Determined by their Eisenstein Spectra (DES). Recall that a signed digraph is said to be determined by its $\mathcal{E}$-spectrum if it is switching isomorphic to every signed digraph to which it is cospectral; see Definitions 1.7 and 1.8 for formal statements.

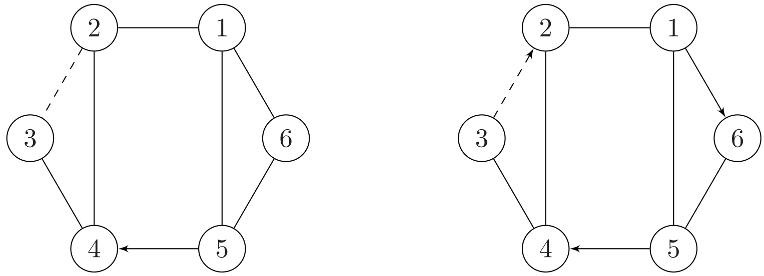
Naturally, we would like to have a way to conclusively determine whether or not a given pair of signed digraphs is switching isomorphic, which is found in [92]. Specifically, Reff [92] presents a sufficient condition, based on the idea (originally from [110]) that the gain of a given cycle in a gain graph is not affected by switching operations. (See Section 1.1.4 for an introductory discussion regarding the relation of cycle gains and the spectrum.) This condition is, in fact, also necessary; a fact previously discussed by Samanta and Kannan [96]. The author feels that the result follows more directly than the discussion in [96] suggests. We present the alternative proof below.

Proposition 4.3. *Let D and Φ be signed digraphs on the graph G. Then $D \sim \Phi$ if and only if there is a D' isomorphic to D with $\varphi(D'[C]) = \varphi(\Phi[C])$ for every cycle C in G.*

Proof. Sufficiency is shown in Reff [92], so we will only discuss necessity. Let $\mathcal{E}(\Phi) = X\mathcal{E}(D)X^{-1}$, and let $C = \{u_1u_2, u_2u_3 \ldots, u_ku_1\}$ be a cycle in G. Then:

$$\begin{aligned}
\varphi_\Phi(C) &= \mathcal{E}(\Phi)_{u_1,u_2}\mathcal{E}(\Phi)_{u_2,u_3}\cdots\mathcal{E}(\Phi)_{u_k,u_1} \\
&= X_{u_1,u_1}\mathcal{E}(D)_{u_1,u_2}X^{-1}_{u_2,u_2}\cdot X_{u_2,u_2}\mathcal{E}(D)_{u_2,u_3}X^{-1}_{u_3,u_3}\cdots X_{u_k,u_k}\mathcal{E}(D)_{u_k,u_1}X^{-1}_{u_1,u_1} \\
&= X_{u_1,u_1}\mathcal{E}(D)_{u_1,u_2}\mathcal{E}(D)_{u_2,u_3}\cdots\mathcal{E}(D)_{u_k,u_1}X^{-1}_{u_1,u_1} \\
&= \varphi_D(C).
\end{aligned}$$

Finally, observe that a relabeling of the vertices changes nothing except for the indices in the above, and the claim follows. $\square$



(a) Φ_a **(b)** Φ_b

Figure 4.2 – Cospectral but not switching isomorphic signed digraphs on one underlying graph.

Marginally expanding on the above, Samanta and Kannan [96] show that one only needs the fundamental cycles of a gain graph to have equal (real parts of) gains. Indeed, it stand to reason that if a basis of the cycle space has equal gains, then all cycles in the cycles space agree. To see this, one simply needs to observe that any cycle C may be obtained as the symmetric difference of fundamental cycles, and note that the gain of C is simply the product of the gains of these fundamental cycles. In this last respect, one should exercise some care, as the traversal direction does matter here, and should be chosen such that the edges on which the fundamental cycles intersect are traversed in opposite directions.

We conclude this section with an application of the above, which shows that cospectral signed digraphs on the same underlying graph may belong to distinct switching isomorphism classes.

Example 4.1. *Consider the signed digraphs Φ_a and Φ_b in Figure 4.2. A quick computation of the characteristic polynomial of their respective Eisenstein matrices yields that*

$$\chi_{\Phi_a}(\lambda) = \chi_{\Phi_b}(\lambda) = \lambda^6 - 8\lambda^4 + 13\lambda^2 - 5.$$

However, the gains of their fundamental cycles, shown in Table 4.1, do not coincide. Thus, Φ_a and Φ_b do not belong to the same switching isomorphism class. As a final note, we remark that this conclusion could also have been drawn by computing the gain of the (sole) 6-cycle in Φ_a and Φ_b, though an application of Proposition 4.3 seems appropriate.

U	$\mathrm{Re}\,(\phi(\Phi_a[U]))$	$\mathrm{Re}\,(\phi(\Phi_b[U]))$
$\{2,3,4\}$	-1	$-1/2$
$\{1,5,6\}$	1	$1/2$
$\{1,2,4,5\}$	$1/2$	$1/2$

Table 4.1 – Fundamental cycle gains in Figure 4.2

4.2.4 Limiting degrees of freedom

As a direct consequence of the equivalence relations discussed before, any exercise in classification of signed digraphs would encounter an abundance of seemingly distinct digraphs, that turn out to be equivalent upon closer inspection. Thus, it is desirable to consider ways to limit the number of possibilities that have to be considered. It seems particularly practical to be able to fix a subset of the edges to a certain type, while maintaining the certainty that all switching isomorphic classes were considered.

In the below, we will show that any switching isomorphism class on a graph G contains at least one member whose edge-induced subdigraph coincides with a fixed spanning tree T of G. This idea is quite natural from a gain graph perspective, using the well-known result that appears here as Corollary 4.4.2. In the interest of completeness, we include a brief proof to a result that will frequently be applied, later on.

Proposition 4.4. *Let G be a graph and let Φ_1, Φ_2 be distinct signed digraphs on G. Let $T \subseteq E(G)$ be a spanning tree of G. Then, there exists a switching matrix Y such that Φ_2', obtained from Φ_2 as $\mathcal{E}(\Phi_2') = Y\mathcal{E}(\Phi_2)Y^{-1}$, satisfies $\Phi_2'[T] = \Phi_1[T]$.*

Proof. Consider the edge $(u,v) \in T$. Since T is a spanning tree, $T \setminus (u,v)$ induces an (edge-induced) subdigraph on G that consists of two disjoint components, say V_1 (that contains u) and V_2 (that contains v); see Figure 4.3. Now, let $\mathcal{E}(\Phi_j)_{uv}$ denote the (u,v) entry of the Eisenstein matrix corresponding to Φ_j, and construct the diagonal matrix $X^{(uv)}$ as

$$X_{jj}^{(uv)} = \begin{cases} \mathcal{E}(\Phi_1)_{uv}/\mathcal{E}(\Phi_2)_{uv} & \text{if } j \in V_1 \\ 1 & \text{if } j \in V_2 \end{cases} \tag{4.1}$$

Now, consider the switched digraph Φ_2', whose Eisenstein matrix is defined as $\mathcal{E}' := X^{(uv)}\mathcal{E}(\Phi_2)\left(X^{(uv)}\right)^{-1}$. Firstly, observe that we have $\mathcal{E}'_{uv} = \mathcal{E}(\Phi_1)_{uv}$, by construction. Moreover, since for any $(p,q) \in T \setminus (u,v)$ it holds that either $\{p,q\} \subset V_1$ or $\{p,q\} \subset V_2$, it follows that $\mathcal{E}'_{pq} = \mathcal{E}(\Phi_2)_{pq}$. In other words, the arcs in Φ corresponding to exactly

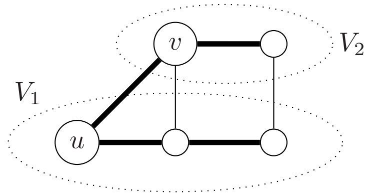


Figure 4.3 – An example graph G for Prop. 4.4. Here, the thick lines represent T.

one edge in T, namely (u, v), were changed by the switching with $X^{(uv)}$. It follows that $Y := \prod_{(u,v) \in T} X^{(uv)}$ satisfies the desired requirements. $\square$

The below conclusions then follows immediately.

Corollary 4.4.1. *Let G be a graph and let $T \subseteq E(G)$ be a spanning tree on G. Further, let $\mathcal{D}$ denote the collection of all signed digraphs on G, and let $\mathcal{D}_T \subset \mathcal{D}$ be the collection of such signed digraphs that coincide with T on the relevant edges. Then*

$$\Phi \in \mathcal{D} \iff \exists \Phi' \in \mathcal{D}_T \text{ s.t. } \Phi \sim \Phi'.$$

The following well-known fact also follows immediately from Proposition 4.4.

Corollary 4.4.2. *Let G be a forest and let $\Phi = (G, \varphi)$ be a signed digraph. Then $\Phi \sim G$.*

Note that $\mathcal{D}_T$ may contain more than one member from a given switching isomorphism class, as illustrated in the following example.

Example 4.2. *Consider the non-isomorphic signed digraphs Φ and Φ', as illustrated in Figures 4.4a and 4.4b, respectively. It is obvious that a tree, represented by the thick lines, coincides. However, if the vertically oriented digons in Figure 4.4b are multiplied by -1 (which clearly is a switching operation), the result is isomorphic to Figure 4.4a. Thus, Φ and Φ' belong to the same switching isomorphism class.*

As a closing remark to this section, we would like to express interest in the non-trivial question that follows up on the example above, and asks exactly how many members of a given switching equivalence class may coincide in a predetermined spanning tree. This matter is not explored further in this work.

(a) Φ (b) Φ'

Figure 4.4 – Signed digraphs for Example 4.2.

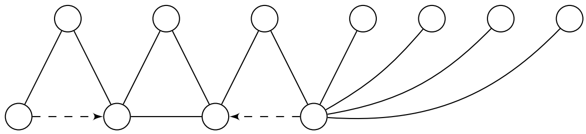


Figure 4.5 – Another signed digraph whose spectrum is symmetric.

4.2.5 Symmetric spectra

In spectral graph theory, it is commonly asked which structural characteristics imply symmetry of the corresponding spectrum. It is well-known that graphs have symmetric spectra if and only if they are bipartite. With respect to the (conventional) Hermitian adjacency matrix H [51], digraphs have been shown to have symmetric spectra if they are bipartite or (switching equivalent to) an oriented[3] digraph, but the reverse implications do not hold. In the current context, one may show the following.

Lemma 4.5. *Let G be a bipartite graph and let $\Phi = (G, \varphi)$ be a signed digraph. Then the spectrum of Φ is symmetric around zero.*

Proof. Let $\Phi' = (G, \varphi')$, where $\varphi'(uv) = -\varphi(uv)$. If G is bipartite then every cycle C of G satisfies $\varphi'(C) = (-1)^{|C|}\varphi(C) = \varphi(C)$. By Proposition 4.3, we thus have $\Phi' \sim \Phi$. Finally, since $\mathcal{E}(\Phi') = -\mathcal{E}(\Phi)$ and their spectra coincide, it follows that said spectra are symmetric. $\square$

However, an oriented signed digraph in general does not have a symmetric spectrum, and no necessary properties were found. As a consequence of the existence of sporadic, 'ugly' examples such as the signed digraph in Figure 4.5, the author expects that a tight characterization of all signed digraphs that have symmetric spectra is unlikely to be found. For further details, Chapter 6 contains an extensive discussion of gain graphs with symmetric spectra.

[3] A digraph is said to be oriented if it contains no digons.

4.3 Signed digraphs of low rank

As we work our way towards spectral characterizations, we first consider signed digraphs of rank 2 or 3. This restriction severely limits the combinatorial complexity of the corresponding structure. Indeed, if almost all rows of its Eisenstein matrix $\mathcal{E}$ need to be linearly dependent, it stands to reason that many vertices have similar relations to one another, as well. Without too much effort, one may show the following two results, regarding the ranks of some basic digraphs.

Lemma 4.6. *Let P_n be a path of order n. Then $\Phi = (P_n, \varphi)$ has rank $2\lfloor n/2 \rfloor$ for any φ.*

Proof. Since $\Gamma(\Phi)$ is a tree, $\text{Rank}\,(\Phi) = \text{Rank}\,(\Gamma(\Phi)) = \text{Rank}\,(P_n)$, by Corollary 4.4.2. □

Lemma 4.7. *Let C_n be a cycle of order n, with n odd. Then $\Phi = (C_n, \varphi)$ has rank n for any φ.*

Proof. C_n has exactly one elementary spanning subgraph, so its characteristic polynomial $\chi(\lambda)$ has a nonzero coefficient a_n, by Theorem 1.3, and thus no zero roots. □

Note that for n even, it also follows that signed digraphs on C_n have rank n, except when they have gain 1 and n is divisible by 4, or when they have gain -1 and $n-2$ is divisible by 4. The case $n = 4$ will be relevant later on.

We note explicitly that since bipartite signed digraphs have symmetric spectra, their ranks are necessarily even. Finally, an intuitive observation, concerning the rank of some block matrices, is the following.

Lemma 4.8. *Let A be a Hermitian matrix defined as*

$$A = \begin{bmatrix} O & A_{12} \\ A_{12}^* & A_{22}. \end{bmatrix},$$

with A_{12} nonzero and where A_{22} has a zero diagonal. If Rank $A = 3$ then Rank $A_{12} = 1$ and $2 \leq$ Rank $A_{22} \leq 3$. Moreover, if Rank $A = 2$ then Rank $A_{12} = 1$ and $A_{22} = O$.

Specifically, the lemma above implies that if two vertices are twins in an induced subdigraph of a signed digraph whose rank is 2 or 3, then they are also twins in said (larger) signed digraph.

4.3.1 Rank 2

Let us first consider signed digraphs of rank 2. As is common in this type of research, the eigenvalue interlacing theorem is used extensively, to forbid particular structures from occurring as induced subgraphs. Using the lemmas above, we may characterize the underlying graphs of all signed digraphs with rank 2, based on this idea.

Lemma 4.9. *If $\Phi = (G, \varphi)$ is a connected signed digraph with Eisenstein rank 2, then G is a complete bipartite graph.*

Proof. By contradiction. By Lemma 4.7, Φ is odd-cycle-free, and thus bipartite. Let P, Q denote the coloring classes of Φ. Now, suppose to the contrary that $u \in P,\ v \in Q$ are a pair of vertices that is nonadjacent in G. Since Φ is connected, there is a $u \to v$ path in G. Let $U \subseteq V(\Phi)$ be the collection of vertices that is traversed on a shortest $u \to v$ path; then $G[U \cup \{u, v\}] \cong P_{2k}$, for some $k > 1$. However, since Rank $P_{2k} = 2k$, we obtain a contradiction, by interlacing. □

The next natural question to ask would be which signed digraphs on underlying graph $K_{p,q}$ have Eisenstein rank 2. In the below, we show that any signed digraph that satisfies this requirement is switching isomorphic to its underlying graph.

Proposition 4.10. *If $\Phi = (G, \varphi)$ is a connected signed digraph with Eisenstein rank 2, then Φ is switching isomorphic to the complete bipartite graph G.*

Proof. By Lemma 4.9, G is complete bipartite. Let P, Q denote the coloring classes, as before. By Proposition 4.4, we may without loss of generality choose the edge gains of a spanning tree of G. If $u \in P$ and $v \in Q$, then such a spanning tree (say, T) may be obtained by taking all edges incident to at least one of u or v. If we choose the edges in T to be positive digons, the Eisenstein matrix $\mathcal{E}(\Phi)$ contains

$$\left[\begin{array}{cc:cc} & & 1 & \mathbf{j}^\top \\ & & \mathbf{j} & X \\ \hdashline 1 & \mathbf{j}^\top & & \\ \mathbf{j} & X^* & & \end{array}\right], \tag{4.2}$$

where the diagonal blocks are square all-zero blocks of appropriate dimensions, $\mathbf{j}$ denotes an all-ones vector and the X blocks are unknown. Finally, since all of the induced 4-cycles must have gain 1, we have

$$\mathcal{E}(\Phi) = \begin{bmatrix} O_{p\times p} & J_{p\times q} \\ J_{q\times p} & O_{q\times q} \end{bmatrix}.$$

Thus, there is exactly one rank 2 switching isomorphism class on $K_{p,q}$, and the claim follows. □

Note that implicitly, all connected rank-2 digraphs have underlying graphs that are twin expansions of K_2. We will see a similar trend if the rank is increased.

4.3.2 Rank 3

Increasing the allowed rank just slightly still allows for a neat characterization of the switching isomorphism classes. To obtain this characterization, we first obtain an understanding of the twin reduced structure, after which expansions and signatures are included.

Proposition 4.11. *Let Φ be a connected, twin reduced signed digraph of order 4 and rank 3. Then $\Phi \sim (T_4, \pm)$,[4] where T_4 denotes the order-4 transitive tournament.*

Proof. Observe that Φ is not bipartite, as bipartite signed digraphs have even rank. Thus, Φ contains an odd-sized cycle, which implicitly is a triangle. Moreover, by connectedness, at least one vertex (say, s) in said triangle is also adjacent to the fourth vertex. We apply Proposition 4.4 to assume without loss of generality that the arcs incident to s have gain 1; that is

$$\mathcal{E}(\Phi) = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & a & \bar{c} \\ 1 & \bar{a} & 0 & b \\ 1 & c & \bar{b} & 0 \end{bmatrix},$$

for $a \in \mathbb{T}_6$ and $b, c \in \mathbb{T}_6 \cup \{0\}$. (Note that a, b, and c are symmetric, so we may assume w.l.o.g. that a is nonzero.) Now, note that if $\operatorname{Re}(a) > 0$ and $\operatorname{Re}(b) < 0$, then by interlacing, Φ has two positive and two negative eigenvalues, and thus $\operatorname{Rank} \mathcal{E}(\Phi) = 4$, and similarly for the pairs b, c and a, c. Thus, a, b, c must be such that either their real parts are all positive or all negative; we assume positivity for now. For a, b, c as

[4] Note that the (D, ϕ) notation is used in this instance, as opposed to (G, φ).

above, we then find that

$$\det \mathcal{E}(\Phi) = 1 + |b| + |c| - 2\mathrm{Re}\,(ab + ac + bc)\,. \tag{4.3}$$

We proceed to distinguish three cases.

(i) $b = c = 0$. Then $\det \mathcal{E}(\Phi) = 1$ and $\mathrm{Rank}\,(\Phi) = 4$.

(ii) $b \neq 0$, $c = 0$. Then $\det \mathcal{E}(\Phi) = 2 - 2\mathrm{Re}\,(ab) = 0 \iff a = \bar{b}$, which implies that Φ is not twin reduced, contradiction.

(iii) $b, c \neq 0$. Then we need $\det \mathcal{E}(\Phi) = 3 - 2\mathrm{Re}\,(ab + ac + bc) = 0$, which holds if and only if one of the following cases is true: (I) $\mathrm{Re}\,(ab) = \mathrm{Re}\,(bc) = \mathrm{Re}\,(ac) = 1/2$ or (II) $\mathrm{Re}\,(ab) = \mathrm{Re}\,(bc) = 1 \ \wedge\ \mathrm{Re}\,(ac) = -1/2$. In case (I), we write $ab = \omega^{k_a + k_b}$, and use that $\mathrm{Re}\,(ab) = 1/2$ implies $k_a + k_b$ is odd. Clearly, there are no integers k_a, k_b, k_c such that $(k_a + k_b), (k_b + k_c)$ and $(k_a + k_c)$ are all simultaneously odd, so the desired a, b, c do not exist. in case (II), assume $\mathrm{Re}\,(a)\,, \mathrm{Re}\,(b)\,, \mathrm{Re}\,(c) > 0$ to conclude that either $a = c = \omega$ and $b = \overline{\omega}$ or $a = c = \overline{\omega}$ and $b = \omega$. Both possibilities are equivalent, and yield $\Phi \sim (T_4, +)$.

Finally, note that if negativity was assumed, we would have obtained $\Phi \sim (T_4, -)$. □

Now, we may naturally try to increase the order. A well-known fact is the following.

Lemma 4.12. *A digraph D is a transitive tournament if and only if every one of its induced subdigraphs is also a transitive tournament.*

The above holds analogously when switching is allowed. We forego a formal proof, as this fact should be clear by observing that the gains of a basis of the cycle space is known and a quick application of Proposition 4.3.

Now, if we extend the above by considering rank-3 signed digraphs of order $n \geq 5$, we find that such signed digraphs are not twin reduced.

Lemma 4.13. *Let Φ be a connected signed digraph of order ≥ 5, rank 3. Then Φ is not twin reduced.*

Proof. Let $n \geq 5$ and suppose to the contrary that Φ is twin reduced, of order n and rank 3. We distinguish three cases.

(i) There is an order-4 induced subdigraph Φ' of Φ such that $\Gamma(\Phi') \cong K_{1,1,2}$. This induced subdigraph has rank at most 3, by interlacing, and is therefore not twin reduced, by Proposition 4.11. Then, using Lemma 4.8, we obtain that the vertices that are twins in Φ' are also twins in Φ, and thus Φ is not twin reduced, contradiction.

(ii) There is an order-4 subdigraph of rank 2 or 0. These are respectively complete bipartite or empty, and therefore contain twins; the contradiction follows as in case (i).

(iii) All order-4 subdigraphs satisfy Proposition 4.11. Then, by interlacing, they are either all switching isomorphic to $(T_4, +)$ or all to $(T_4, -)$. Hence, using Lemma 4.12, we find $\Phi \sim (T_5, \pm)$. However, Rank $(T_5, \pm) = 5$, and we obtain a contradiction.

All three possible cases yield a contradiction, so the claim follows. □

The results above show that the number of distinct structures (up to switching isomorphism) whose clique expansions have rank 3 is very small. Thus, we easily arrive at the following result, that concerns their expanded counterparts.

Proposition 4.14. *Let Φ be a connected signed digraph of rank 3. Then either $\Phi \sim TE((K_3, \varphi), \tau)$, for any φ and $\tau \in \mathbb{N}^3$, or $\Phi \sim TE((T_4, \pm), \tau)$, $\tau \in \mathbb{N}^4$.*

Proof. Note that any triangle has rank 3, and observe that any complete tripartite signed digraph has rank 3 if and only if the edges between partition groups have equal types, as touched upon in the proof of Lemma 4.11. The second part of the claim then follows by application of Lemmas 4.11 and 4.13. □

4.4 Few non-negative eigenvalues

Inspired by the recent work by Oboudi [87], we inquire into signed digraphs that satisfy a different set of spectral requirements. Specifically, we now require candidates to have an (almost) minimal number of non-negative or, equivalently, non-positive eigenvalues. A neat characterization of signed digraphs that admit to these conditions, could be the foundation upon which to build another set of (possibly infinite) families of signed digraphs, whose spectra determine them, up to switching isomorphism.

Until the end of this section, we will consider the former case, that is, few strictly positive eigenvalues. However, note that the negative case is indeed equivalent, and may be obtained by multiplying the signature φ by -1. Additionally, observe that (switching) twins are inherently forbidden, since their existence implies the occurrence of 0 as an eigenvalue.

4.4.1 One non-negative eigenvalue

A clear starting point for this investigation is the class of signed digraphs with exactly one non-negative eigenvalue.

Proposition 4.15. *The signed digraph $\Phi = (G, \varphi)$ satisfies $\lambda_2 < 0$ only if G is complete.*

Proof. By induction on the order n of Φ. For $n = 2$, the claim is obviously true. Now, suppose that the claim holds for any order-n signed digraph Φ, and consider Φ' of order $n+1$. Since the underlying graph of every order-n induced subgraph of Φ' is complete, by the induction hypothesis and eigenvalue interlacing, it follows that $\Gamma(\Phi')$ is complete. □

We note explicitly that Proposition 4.15 is not sufficient. One may, for example, consider the signed digraph $(T_4, +)$, which has $\lambda_2 = 0$, while its underlying graph is complete.

Building on Proposition 4.15, we will now characterize all signed digraphs whose second largest eigenvalue is negative. Indeed, note that we thus far know for sure that such a signed digraph must have a complete underlying graph, but which (and how many) signatures φ may be added to yield a signed digraph that satisfies the desired spectral requirements, is as of yet unknown. In the below, we find that this collection is limited to exactly two switching equivalence classes, for given n.

Definition 4.3. *Let K_n^* denote the digraph obtained from K_n by orienting exactly one edge.*

Lemma 4.16. *K_n^* has a negative second-largest eigenvalue for all $n \geq 3$.*

Proof. The characteristic polynomial of K_n^* is given by

$$\chi(\lambda) = (\lambda+1)^{n-3}\left(\lambda^3 - (n-3)\lambda^2 - (2n-3)\lambda - 1\right),$$

which by Descartes rule of signs has exactly one positive root, and clearly no zero roots. □

Theorem 4.17. *Let Φ be a signed digraph with $\lambda_2 < 0$. then either $\Phi \sim K_n$ or $\Phi \sim K_n^*$.*

Proof. By Proposition 4.15, $\Gamma(\Phi)$ is complete. Then, the claim may easily be verified for $n \leq 4$, and we proceed by induction. Let $n \geq 4$, suppose that the claim is true for signed digraphs of order n and consider a signed digraph Φ of order $n+1$. Let k denote the number of such induced subdigraphs that are switching isomorphic to K_n, and let $V := V(\Phi')$.

Note that the $n+1$ order-n induced subdigraphs of Φ must all simultaneously satisfy $\lambda_2 < 0$, by eigenvalue interlacing. This implies that every such order-n subgraph has either only gain-1 triangles, or has $n-2$ triangles whose gain is ω, which all intersect on an edge, and $\binom{n}{3} - n + 2$ gain-1 triangles.[5]

Now, we may count the number of pairs (u, t) where $u \in V(\Phi)$ is not part of the gain-ω triangle t in Φ. Since for all $u \in V$ we have $\Phi[V \setminus \{u\}] \cong K_n$ or K_n^*, where the former holds for k out of the $n+1$ order-n subgraphs, we find that there are $(n+1-k)(n-2)$ such pairs (u, t). Similarly, since every gain-ω triangle contains all but $n-2$ vertices of Φ, there are $(n-2)\Delta$ such pairs, where Δ is the total number of gain-ω triangles in Φ. Hence, $\Delta = n + 1 - k$.

Now, we may distinguish a few cases. If $k \geq 4$, then every triangle in Φ is part of at least one induced subgraph that is switching isomorphic to K_n, and thus $T = 0$, which implies $k = n+1$ and thus $\Phi \sim K_{n+1}$. Similarly, if $k = 3$, then all but one triangle in Φ certainly have gain 1. This implies $\Delta \leq 1$ and thus $n \leq 3$, which is a contradiction.

If $k = 2$, then $\Delta = n-1$. Suppose that $\Phi[V \setminus \{u\}]$ and $\Phi[V \setminus \{v\}]$ are the $\sim K_n$ subdigraphs. Then at most the triangles that contain the edge (u, v) may have gain ω; the others all have gain 1. Moreover, since there are exactly $n-1$ such triangles, all of them necessarily have gain ω. Then, using that the collection of triangles in a complete graph form a basis of the cycle space, we may apply Proposition 4.3 to conclude that $\Phi \sim K_n^*$.

Next, if $k = 1$ then $\Delta = n$. Suppose that $\Phi[V \setminus \{u\}] \sim K_n^*$. Then, the $n-2$ gain-ω triangles in $\Phi[V \setminus \{u\}]$ intersect on some edge (v, z). Moreover, at least one of $\Phi[V \setminus \{v\}]$ and $\Phi[V \setminus \{z\}]$ is also switching equivalent to K_n^*, which thus contains $n-2$ different gain-ω triangles, necessarily containing u. Hence, $n = \Delta \geq 2(n-2)$, which implies $n \leq 4$ and thus $n = 4$. This yields the potential counterexample $\Phi \sim K_5^{**}$,

[5] Recall that a cycle is said to have gain ω if taking the product of the arc gains corresponding to the arcs hit by traversal of the cycle in at least one direction equals ω. I.e., $\varphi(C) = \omega$ if either $\varphi(C^{\rightarrow})$ or $\varphi(C^{\leftarrow})$ equals ω.

where K_5^{**} is obtained from K_5 by orienting two of its edges, such that their initial vertex coincides. However, a quick computation of its spectrum yields $\lambda_2 = 0$, and thus K_5^{**} does not satisfy the claim.

Finally, if $k = 0$ then $\Delta = n + 1$, which, as above, implies that $n + 1 \geq 3(n - 2)$ and thus $n \leq 3$, which is a contradiction. $\square$

As was previously mentioned, Theorem 4.17 tells us that for a given order n, a signed digraph that satisfies $\lambda_2 < 0$ must belong to exactly one of two (spectrally distinct, recall Lemma 4.2) switching isomorphism classes. This ties in to a natural spectral characterization result, which is provided in Section 4.5.

To conclude this section, we briefly discuss the natural question how much of the above carries over when instead, signed digraphs with one *positive* eigenvalue are considered; that is, when zero eigenvalues are allowed. It turns out that the collection of (twin reduced) signed digraphs with this property contains various ('ugly') members of increasing order, that have little in common with the families of graphs that have been discussed so far. As such, this is considered out of the scope of this work.

4.4.2 Signed digraphs with $\lambda_2 > 0 > \lambda_3$

In a recent article, Oboudi [87] characterized all graphs with exactly two non-negative eigenvalues. This collection turns out to be an exhaustive list of fairly reasonable length. As such, it seems reasonable to ask whether an analogue idea may be applied in the current context. In this section, we will first find some necessary structural properties, to which any signed digraph that satisfies $\lambda_2 > 0 > \lambda_3$ must admit. After that, we will inquire into the signatures of signed digraphs on such graphs.

Necessary properties

The original result by Oboudi [87] follows quite straightforwardly as a forbidden subgraph result that forbids O_3 and C_4. Clearly, O_3 should still be forbidden, as its inclusion would imply a non-negative third-largest eigenvalue, by eigenvalue interlacing. However, since a signed digraph on C_4 still meets the requirements if its gain is not 1, we must substantially deviate from the conclusions in [87]. As usual, let us first consider the graph structures that may be underlying to signed digraphs that satisfy our needs.

Lemma 4.18. *Let G be a connected O_3-free graph, of order $n \geq 5$. Every order-5 vertex-induced subgraph contains a C_5 or a clique expansion of P_4.*

It should be noted that the collection of graphs that are O_3-free contains many graphs with higher edge-density than clique expansions of C_5 and P_4. However, as should be clear to the reader, given such a graph, one may always remove edges to arrive at a graph that is still O_3-free, but which *is* such an expansion. That is to say, a graph is O_3-free *because* every relevant subset of the vertices is contained in either one of C_5, P_4, or a clique.

Given the above, we may formulate some natural conditions for a signed digraph to satisfy $\lambda_2 > 0 > \lambda_3$. These will be particularly useful in Section 4.5, when we are constructing potential cospectral mates of a given signed digraph.

Proposition 4.19. *Let $\Phi = (G, \varphi)$ be a connected signed digraph that satisfies $\lambda_2 > 0 > \lambda_3$. Then G is a clique expansion of P_4 or C_5, possibly supplemented with additional edges up to a complete graph. Additionally, it must satisfy the following:*

(i) For every $U \subset V(\Phi)$ with $\Gamma(\Phi[U]) = K_4$, at least one triangle in $\Phi[U]$ is positive,

(ii) For every $U \subset V(\Phi)$ with $\Gamma(\Phi[U]) = C_4$, it holds that $\varphi(\Phi[U]) \neq 1$,

(iii) For every $U \subset V(\Phi)$ with $\Gamma(\Phi[U]) = C_5$, it holds that $\mathrm{Re}\,(\varphi(\Phi[U])) < 0$,

Proof. Follows from Lemma 4.18 and the forbidden subdigraphs switching isomorphic to (K_4, φ_1), $(C_4, +)$ and (C_5, φ_2), where φ_1 is such that all triangles in K_4 are negative, and φ_2 is such that the 5-cycle has positive gain. □

In case we relax the assumption on connectedness, the following conclusion is an immediate consequence of Theorem 4.17.

Proposition 4.20. *Let Φ be a signed digraph on G, where G is a graph that is obtained as the disjoint union of at least two connected components. If Φ satisfies $\lambda_2 > 0 > \lambda_3$ then $\Phi = \Phi_1 \cup \Phi_2$, where $\Phi_j \sim K_{n_j}$ or $\Phi_j \sim K^*_{n_j}$, $j = 1, 2$.*

The conditions in Proposition 4.19 are certainly not sufficient; plenty of examples to show this are provided in Figures 4.6, 4.7 and 4.9, as well as any clique expansions of C_5that exceed Table 4.2.

Due to an abundance of possibilities, the full classification of signed digraphs with $\lambda_2 > 0 > \lambda_3$ is not provided here. However, we will still zoom in on a few special cases. While the complete graph seems like an attractive starting point, the vast number of admissible signatures drove the author to first consider more palpable families. In particular, we will investigate a selection of the clique expansions of P_4 and C_5, which in a sense have the minimal required number of edges. In the remainder of this section, we will classify such signed digraphs that satisfy $\lambda_2 > 0 > \lambda_3$; these families will be revisited in Section 4.5, where we provide spectral characterizations.

Short kite graphs

An (a, b)-kite is said to be obtained from a K_a and a P_b by connecting some vertex in the clique to a pendant vertex of the path. Such graphs have recently been shown to be determined by their adjacency spectra, for all choices of a and b [99]. Moreover, if $b = 1$ or $b = 2$, then for any $a \geq 2$, the corresponding (a, b)-kite graph is O_3-free, and may potentially satisfy $\lambda_2 > 0 > \lambda_3$. In fact, we obtain a rather nice parallel to the results of Section 4.4.1. It seems intuitive that the complete part of the kite should have a negative second largest eigenvalue, in order for the corresponding signed digraph to satisfy $\lambda_2 > 0 > \lambda_3$. An elegant application of eigenvalue interlacing confirms this belief.

Proposition 4.21. *Let $\Phi = (K_n, \varphi)$, $\mathbf{v} \in \{\mathbb{T}_6 \cup 0\}^n$ and let*

$$\mathcal{E} := \begin{bmatrix} \mathcal{E}(\Phi) & \mathbf{v} & \mathbf{0} \\ \mathbf{v}^* & 0 & 1 \\ \mathbf{0}^\top & 1 & 0 \end{bmatrix}.$$

Then $\mathcal{E}$ satisfies $\lambda_2 > 0 > \lambda_3$ if and only if Φ is switching isomorphic to K_n or K_n^*.

Proof. Since the eigenvalues μ_j of

$$\mathcal{E}' := \begin{bmatrix} \mathcal{E}(\Phi) & \mathbf{0} \\ \mathbf{0}^\top & 0 \end{bmatrix}$$

interlace those of of $\mathcal{E}$, necessity of the claim follows by Theorem 4.17. Indeed, note that $\mu_3 \geq 0$ yields a contradiction, by interlacing.

Now suppose that Φ is switching isomorphic to K_n or K_n^*. Then, again using that the eigenvalues μ_j of $\mathcal{E}'$, which by construction satisfy $\mu_1 > 0 = \mu_2 > \mu_3$, interlace those of $\mathcal{E}$, we obtain $\lambda_1 \geq \mu_1 \geq \lambda_2 \geq 0 \geq \lambda_3$. Finally, observe that

$$\prod_{j=1}^{n+2} \lambda_j = \det \mathcal{E} = -\det \begin{bmatrix} \mathcal{E}(\Phi) & \mathbf{0} \\ \mathbf{v}^* & 1 \end{bmatrix} = -\det \mathcal{E}(\Phi) = \mu_1 \cdot \prod_{j=3}^{n+1} \mu_j \neq 0,$$

and thus $\lambda_2 > 0 > \lambda_3$. $\square$

Since the above is quite independent of the choice of $\mathbf{v}$, the desired result follows easily.

Corollary 4.21.1. *Let Φ be a signed digraph of order $n \geq 5$ whose underlying graph is a $(n-1, 1)$ or $(n-2, 2)$-kite graph. Then Φ satisfies $\lambda_2 > 0 > \lambda_3$ if and only if it contains a subdigraph that is switching isomorphic to K_{n-2} or K_{n-2}^* that is non-adjacent to the pendant vertex.*

Semi-complete signed digraphs

If not one, but instead both pendants of P_4 are expanded, we obtain a convenient structure that contains many induced $(a, 2)$-kites. Thus, if $\lambda_2 > 0 > \lambda_3$ is required, we get substantial structural information almost for free.

Definition 4.4. *Let $G = CE(P_4, [p \quad 1 \quad 1 \quad q])$, $p, q \in \mathbb{N}$ with $p, q \geq 2$, and let $P \subset V(G)$ be the vertices associated with p. Let $\tilde{\varphi}$ be the signature that differs from the all-one signature only on (u, v), $u, v \in P$, which has $\tilde{\varphi}(u, v) = \omega$. Similarly, let $\hat{\varphi}$ be the signature that differs from the all-one signature only on (s, t), $s, t \in Q$, with $\hat{\varphi}(s, t) = \omega$. Then $\tilde{\Phi} := (G, \tilde{\varphi})$ and $\hat{\Phi} := (G, \hat{\varphi})$.*

Proposition 4.22. *Let $p, q \in \mathbb{N}$, let $G = CE(P_4, [p \quad 1 \quad 1 \quad q])$, Then $\Phi = (G, \varphi)$ satisfies $\lambda_2 > 0 > \lambda_3$ if and only if $\Phi \sim G$, $\Phi \sim \tilde{\Phi}$ or $\Phi \sim \hat{\Phi}$.*

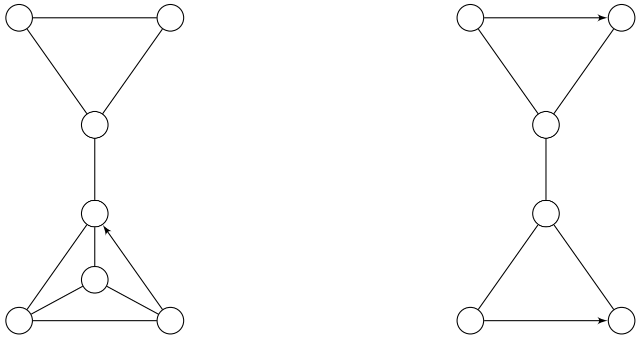
Proof. Necessity follows by a straightforward application of Proposition 4.20, while respecting the forbidden subdigraphs in Figure 4.6.

Now, suppose that $\Phi \sim G$, $\Phi \sim \tilde{\Phi}$ or $\Phi \sim \hat{\Phi}$ which contains respectively $K_{p+1} \cup K_q$, $K_{p+1}^* \cup K_q$ or $K_p \cup K_{q+1}^*$ as an induced subgraph. Since either satisfies $\mu_2 > 0 > \mu_3$ (by Theorem 4.17), we obtain by interlacing that Φ has at most three positive eigenvalues. Then, using some elementary matrix algebra, we find that both cases satisfy

$$\operatorname{sign}(\det \mathcal{E}(\Phi)) = (-1)^{p+q+2}.$$

Hence, its number of positive eigenvalues must be even, and thus be equal to two. □

The G above is a so-called semi-complete graph, which in general consists of two cliques and an arbitrary number of bridges. In his investigation of graphs with at most two non-negative eigenvalues, Oboudi [87] finds that graphs, which satisfy $\lambda_2 > 0 > \lambda_3$, are clique expansions the members of a family of clique reduced semi-complete graphs that are C_4-free.



(a) **(b)**

Figure 4.6 – Two signed digraphs with $\lambda_3 = 0$.

Thus, it would be natural to ask which signed digraphs on semi-complete graphs satisfy $\lambda_2 > 0 > \lambda_3$. Conveniently, we find that the clique reduced graphs in Oboudi's family contain large induced $(n-2,2)$-kite graphs, to which we may apply Corollary 4.21.1 and interlacing to conclude that its complete parts should be switching isomorphic[6] to K or K^*. However, this does not yield much useful information regarding the possible signatures of the bridges. In fact, it turns out that there are admissible signed digraphs on Oboudi's graphs whose triangle gains do not all share the same sign. Moreover, if we generalize from Oboudi's family of graphs, and allow for induced four-cycles, a similar phenomenon occurs. These graphs are illustrated in Figure 4.7.

These potentially occurring negative triangles open up a vast number of potential signatures to consider. Thus, a concise, full classification of the signed digraphs with $\lambda_2 > 0 > \lambda_3$, whose underlying graphs are semi-complete graphs may not exist.

Clique expansions of C_5

By applying what we have learned about kite graphs, we may draw some interesting conclusions with regard to the expansions of C_5. Indeed, it is not hard to see that any clique expansion of C_5 contains many proper induced subgraphs that are simply $(n-2,2)$-kite graphs. Thus, under the usual assumptions (recall Prop. 4.19), we may substantially limit the potential signatures.

In order to structure the following discussion, it is convenient to define some dis-

[6]In case n is even; if n is odd then the situation is slightly more complicated. Here, K and K^* are respectively the complete graph and the signed digraph defined in Definition 4.3, of appropriate order.

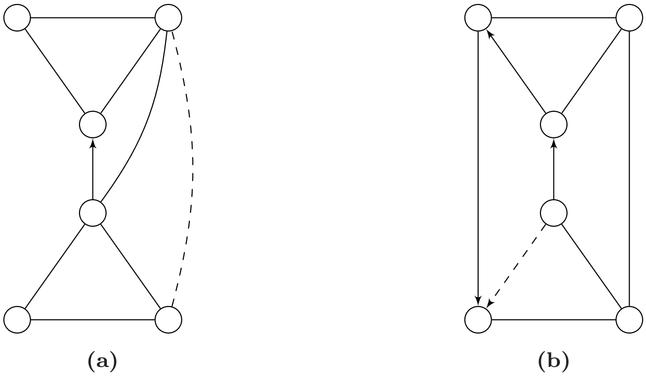


Figure 4.7 – Two semi-complete examples with $\lambda_2 > 0 > \lambda_3$, which contain negative triangles.

tinct types of signatures, for clique expansions of C_5. Given some $G = CE(C_5, \tau)$ and $\Phi = (G, \varphi)$, the four distinct signature types φ are displayed in Figure 4.8. Informally, all induced cliques in types A and C are switching isomorphic to complete graphs, while all of their induced 5-cycles have gains -1 and $-\omega$, respectively. Oppositely, types B and D do contain gain-ω triangles. If the induced cliques associated with expansion parameter τ_j are denoted C_j, then type D is such that exactly one pair (i, j) is such that $C_i \cup C_j$ induces a K^*, while every C_j induces K and the induced 5-cycles have gain 1 or ω. Similarly, expansions of type B are such that exactly one C_j induces a K^*, the remaining four induce K, and all induced 5-cycles have gain 1. We find the following.

Proposition 4.23. *Let G be a clique expansion of C_5, and let $\Phi = (G, \varphi)$ be a signed digraph that satisfies $\lambda_2 > 0 > \lambda_3$. Then $\Phi \sim \Phi' = (G, \varphi')$ where φ' is type A, B, C or D.*

Proof. As usual, we may assume that a spanning tree $Y \subseteq E(G)$ of the edges are positive digons in Φ. Specifically, if we denote the cliques corresponding to expansion coefficient t_j (see Figure 4.8) by G_j, a convenient choice of spanning tree is obtained by fixing five nodes $u_j \in V(G_j)$, $j = 1, \ldots, 5$, and choosing the spanning tree

$$Y = \bigcup_{j=1}^{5} \{(u_j, v) \mid v \in V(G_j) \setminus u_j\} \cup \bigcup_{j=1}^{4} \{(u_j, u_{j+1})\}.$$

Since the subgraph $\Phi[V(G_j) \cup V(G_k)]$ induced by two adjacent cliques, indexed by j, k,

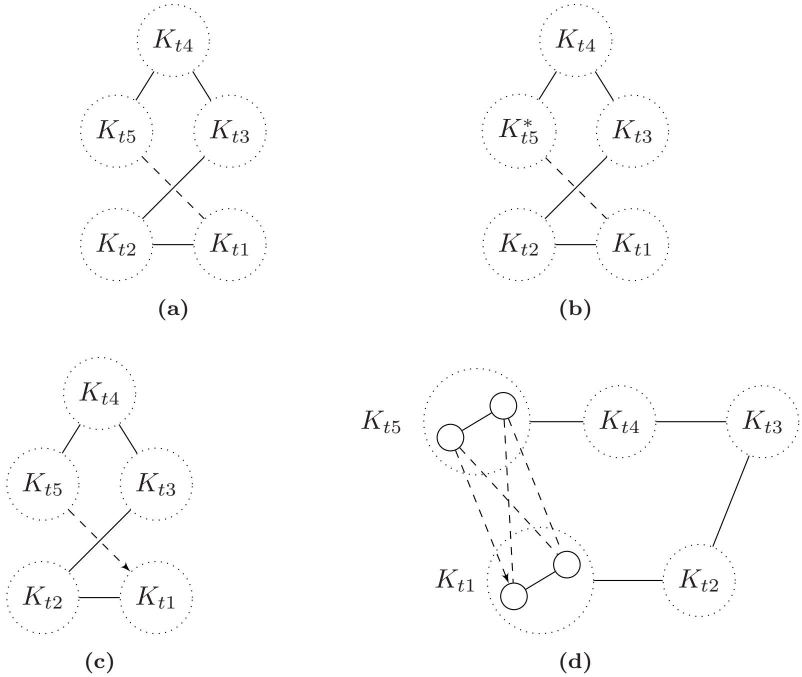
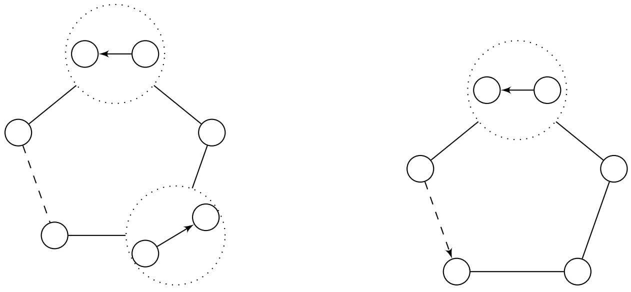


Figure 4.8 – Illustrations of signature types A, B, C, D.

is again a clique, the subgraph $\Phi[V(G_j)\cup V(G_k)]$ necessarily satisfies $\mu_2 < 0$, since the eigenvalues of $\Phi[V(G_j)\cup V(G_k)]\cup O_1$ interlace those of Φ. For such subgraphs with $k = j+1$, $j \in [4]$, we may use that a spanning tree of the induced clique consists of positive digons, to find that exactly one of two cases must be true: either all edges in the induced clique are positive digons, or the induced clique contains exactly one positive arc and the remainder is made up of positive digons. Finally, $\Phi[V(G_1)\cup V(G_5)]$ must also be switching equivalent to either K_m or K^*_m, for appropriate m. However, since every induced C_5 necessarily has negative gain, it follows straightforwardly that the edges between G_1 and G_5 must either be all negative digons, or a single negative arc supplemented with negative digons. Note that either option may indeed be obtained from K_m or K^*_m with a simple diagonal switch that hits the edges between G_1 and G_5.

By the above, no two adjacent G_j may both contain an arc. Thus, natural question would be whether or not two non-adjacent cliques may both contain an arc. Now, since the smallest admissible signed digraph that might satisfy this property, structured as



(a) (b)

Figure 4.9 – Two clique expansions of C_5 with $\lambda_3 = 0$

Figure 4.9a, has a zero third largest eigenvalue, we may conclusively answer this question with 'no.' In a similar vein, since the structure in Figure 4.9b also has $\lambda_3 = 0$, none of the cliques may contain an arc if one of the induced five-cycles has gain $-\omega$. Combining all of the above, we obtain that if $G = CE(C_5, \tau)$ and Φ satisfies $\lambda_2 > 0 > \lambda_3$, then φ must be switching equivalent to a type A, B, C, or D signature. $\square$

However, as was briefly mentioned before, not any clique expansion of C_5 may be underlying to a signed digraph that fits our requirements. Using our knowledge on the admissible signatures, we learn the following by a computer search. In the below, we write $\mathcal{T}_j = \left\{G \cong G'[U] \mid U \subseteq V(G'),\ G' = CE(C_5, \tau^j)\right\}$; that is, $\mathcal{T}_j$ is the collection of all graphs that are obtained from C_5 by clique expansion with expansion vector at most τ^j.

Proposition 4.24. *Let $\Phi = (G, \varphi)$ be a signed digraph that satisfies $\lambda_2 > 0 > \lambda_3$. Then, up to switching equivalence, the following holds:*

(i) if φ is type A, then $G \in \bigcup_{j=1}^{13} \mathcal{T}_j$,

(ii) if φ is type B or D, then $G \in \mathcal{T}_{12} \cup \mathcal{T}_{13}$, and

(iii) if φ is type C, then $G \in \mathcal{T}_{14}$,

where the τ_j are displayed in Table 4.2.

From Table 4.2, we may observe that there are still arbitrarily large expansions of C_5 that satisfy our needs, in addition to some subtly differently structured smaller ones.

φ type:	A											A,B,D		C
	τ^1	τ^2	τ^3	τ^4	τ^5	τ^6	τ^7	τ^8	τ^9	τ^{10}	τ^{11}	τ^{12}	τ^{13}	τ^{14}
t_1	3	3	3	3	4	5	5	5	3	t_1	t_1	t_1	t_1	t_1
t_2	3	3	4	2	2	3	2	1	1	1	t_2	t_2	1	1
t_3	3	2	2	4	2	1	2	3	5	2	2	1	1	1
t_4	2	2	2	2	2	2	2	2	2	2	1	1	t_4	1
t_5	1	2	1	1	2	1	1	1	1	1	2	t_5	t_5	1

Table 4.2 – Maximum clique expansions sizes of C_5, such that it admits a signed graph that satisfies $\lambda_2 > 0 > \lambda_3$. Free variables in τ^{10}-τ^{14} may be arbitrarily large. Note that for types A and D, the collections $\mathcal{T}_{12}$ and $\mathcal{T}_{13}$ are equal. However, since they do not necessarily coincide for type B, the distinction is kept.

It should be noted here, that the signed digraphs obtained by taking a $G \in \mathcal{T}_j$ and an admissible φ from the parameters and structures described above are, as has been the habit throughout, in some sense leading members of a switching equivalence class. For example, if one starts with a C_5 whose gain is $-\omega$, any single vertex may be clique expanded to arbitrary size, without compromising the spectral requirement. However, since every signed digraph obtained in such a manner is switching equivalent to one obtained by expansion of vertex "1," as in Figure 4.8, these are not explicitly listed.

4.5 Cospectrality and determination

Of particular interest to the author are uniquely occurring spectra of graphs. That is, spectra that uniquely determine a graph, up to isomorphism. This notion has received considerable attention for several decades [27, 28]. When an analogous line of research was launched for the Hermitian adjacency matrix H, Mohar [83] subtly shifted the definition of "determined by the spectrum" such that 'DS' digraphs were now allowed to have non-isomorphic cospectral mates, as long as they were all *switching* isomorphic.

In a Chapter 2, we considered the traditional notion, applied in the Hermitian adjacency matrix paradigm. It was determined that digraphs whose H-spectra occur uniquely, up to isomorphism, are extremely rare; though some infinite families do exist. However, we find that with respect to $\mathcal{E}$, any non-empty signed digraph has a (in fact, many) non-isomorphic, switching equivalent partner. This is formally shown below, with an intuitive counting argument. Thereafter, we make use of the classifications from Sections 4.3 and 4.4 to prove that several of the discussed families have spectra that occur only for their respective switching equivalence classes; i.e., these families are determined by their spectra in the broader sense [83].

4.5.1 Existence of a switching equivalent partner

We will formally show that any non-empty signed digraph has at least one switching equivalent, non-isomorphic partner. In the upcoming proofs, let $\Omega_k(\mathcal{E})$ denote the number of entries of $\mathcal{E}$ that are equal to ω^k, for $k \in \mathbb{Z}_6$. We make the following observation.

Lemma 4.25. *Let $\Phi = (G, \varphi)$ be a signed digraph. Let $U \subset V$ and $W = V \setminus U$ be a cut, and partition $\mathcal{E}(\Phi)$ such that*

$$\mathcal{E} = \begin{bmatrix} \mathcal{E}_{U,U} & \mathcal{E}_{U,W} \\ \mathcal{E}_{W,U} & \mathcal{E}_{W,W} \end{bmatrix}.$$

If there are $k, l \in \mathbb{Z}_6$ such that $\Omega_k(\mathcal{E}_{U,W}) \neq \Omega_l(\mathcal{E}_{U,W})$, then there is a $\Phi' \ncong \Phi$ such that $\Phi' \sim \Phi$.

Proof. Suppose that there are $k, l \in \mathbb{Z}_6$ such that $\Omega_k(\mathcal{E}_{U,W}) \neq \Omega_l(\mathcal{E}_{U,W})$ and assume to the contrary that $\Phi' \cong \Phi$ for all $\Phi' \sim \Phi$. Consider the switching matrix

$$S_k = \begin{bmatrix} \omega^k I_u & O \\ O & I_{n-u} \end{bmatrix} \quad \text{with } k \in \mathbb{Z}_6,$$

and set $\mathcal{E}_k = S_k \mathcal{E} S_k^{-1}$, which serves as the Eisenstein matrix of the switching isomorphic signed digraph Φ_k. Since isomorphic signed digraphs necessarily contain an equal number of positive digons, $\Omega_0(\mathcal{E}_k) = \Omega_0(\mathcal{E})$. Note that $\mathcal{E}_{U,U} = (\mathcal{E}_k)_{U,U}$ and $\mathcal{E}_{W,W} = (\mathcal{E}_k)_{W,W}$, and that

$$\Omega_p(\mathcal{E}_{U,W}) = \Omega_{p+k}((\mathcal{E}_k)_{U,W}) \quad \text{for all } p, k \in \mathbb{Z}_6.$$

Then, since $\mathcal{E}, \mathcal{E}_k$ are Hermitian, it follows that $\Omega_0(\mathcal{E}_{U,W}) = \Omega_0(\mathcal{E}_k)_{U,W} = \Omega_{-k}(\mathcal{E}_{U,W})$ for every $k \in \mathbb{Z}_6$ and we obtain a contradiction. □

Now, we may simply consider the number of edges that is hit by a given cut, to determine that the required cut U and k, l certainly exist in a given non-empty signed digraph.

Proposition 4.26. *Let Φ be non-empty. Then there exists a $\Phi' \ncong \Phi$ such that $\Phi \sim \Phi'$.*

Proof. Let Φ be a non-empty signed digraph, and suppose that Φ is strongly determined by its spectrum. Then, for any cut $U \subset V(D)$ and any switching over the edges between U and $V(\Phi) \setminus U$, the digraph obtained by the corresponding switching is isomorphic to Φ. By Lemma 4.25, this implies that any cut of Φ hits equally many edges of every type. This, in turn, implies that any cut in $\Gamma(\Phi)$ must hit a number of edges that is divisible by 6.

Now, suppose that u, v are two vertices that are neighbors in $\Gamma(\Phi)$. By the above, the degrees d_u and d_v of u and v, respectively, must satisfy $d_u \equiv 0 \pmod 6$ and $d_v \equiv 0 \pmod 6$. But then the cut set $\{u, v\}$ hits exactly $d_u + d_v - 2 \equiv 4 \pmod 6$ edges, and we have a contradiction. $\square$

To conclude, we remark that the line above holds for any finite unit gain group except $\mathbb{T}_2$. However, if the the set of allowed complex unit gains is not closed under multiplication, one may construct examples such that each cut that violates the premise above does not allow for gain switching, and therefore cannot produce a counterexample. This phenomenon occurs, for example, with the Hermitian adjacency matrix for directed graphs, and is exploited in Chapter 2.

4.5.2 Spectral determination

By the conclusion in the previous section, it is natural to adopt the before mentioned definition of spectral determination due to Mohar. Formally, we have the following.

Definition 4.5. *[83] Let Φ be a signed digraph and let $Co(\Phi)$ be the collection of signed digraphs whose spectra coincide with the spectrum of Φ. Φ is said to be determined by its $\mathcal{E}$-spectrum (DES) if $\Phi \sim \Phi'$ for all $\Phi' \in Co(\Phi)$.*

In the remainder of this work, we draw from the classifications in Sections 4.3 and 4.4 and verify whether or not some of these families, whose spectral behaviour is, in a sense, extreme, have non-equivalent cospectral mates.

Low rank

Let us first consider the families of signed digraphs with low rank. Since the collection of graphs that might be underlying to such signed digraphs was neatly characterized, we may straightforwardly show the following results.

Proposition 4.27. *Let Φ be a connected signed digraph with Rank$(\Phi) = 2$. If D is connected and cospectral to Φ, then $D \sim \Phi$.*

Proof. Recall from Proposition 4.10 that $\text{Rank}\,(D) = \text{Rank}\,(\Phi) = 2$ implies $\Phi \sim K_{f,g}$ and $D \sim K_{p,q}$, for $f, g, p, q \in \mathbb{N}$. Now, we may simply solve

$$\begin{cases} |V(\Phi)| = |V(D)| \\ |E(\Phi)| = |E(D)| \end{cases} \iff \begin{cases} p + q = f + g \\ pq = fg \end{cases} \iff (p, q) = (f, g) \ \vee (p, q) = (g, f).$$

To obtain $\Phi \sim K_{f,g} \cong K_{p,q} \sim D$, which completes the proof. □

An important note to place here is that the assumption on connectedness is almost always required. Indeed, note that for instance $K_{1,4}$ and $K_{2,2} \cup K_1$ (known as the saltire pair) admit to the requirements, but are cospectral. The reason is quite simple: if connectedness is relaxed, then one may (using the notation from the proof above) simply find numbers p, q such that $pq = fg$, add r isolated vertices to satisfy $p+q+r = f + g$. The following small generalizations follow straightforwardly from this insight.

Corollary 4.27.1. *Let $\Phi \sim K_{p,q}$ with p, q prime. Then Φ is DES.*

Corollary 4.27.2. *Let $\Phi \sim K_{n,n}$, for $n \in \mathbb{N}$. Then Φ is DES.*

Proof. Follows since Φ attains the minimum number of vertices $(2n)$ necessary for a rank-2 signed digraph with $|E| = n^2$. □

In Section 4.3, we have shown that Φ has rank 3 if and only if its twin reduction is equivalent to either a triangle[7] or an order-4 transitive tournament. However, contrary to the above, their respective expansions may sometimes be cospectral, as was observed in [73]. Cospectrality occurs for each pairing of the positive reduced graphs K_3, K_3^*, T_4, and equivalently for their negative counterparts. The smallest examples to this fact are:

- $TE(K_3, [1\ 8\ 15])$ is cospectral to $TE(K_3^*, [3\ 5\ 16])$,
- $TE(K_3^*, [3\ 4\ 7])$ is cospectral to $TE(T_4, [1\ 1\ 6\ 6])$,
- $TE(K_3, [3\ 20\ 25])$ is cospectral to $TE(T_4, [3\ 5\ 10\ 30])$.

[7] Recall that there are exactly four classes of triangles, which contain K_3, K_3^*, $-K_3$ and $-K_3^*$, respectively.

Moreover, each of the three reduced signed digraphs has an arbitrarily large (nontrivial) twin expansion cospectral to a signed digraph with a different underlying graph. The propositions below are easily checked by simply counting the number of vertices, edges, and triangles[8].

Proposition 4.28. *Let* Φ *and* Φ' *be defined as* $\Phi = TE(K_3^*, [2i+1 \;\; i(3i+2) \;\; 2(3i+1)(i+1)])$ *and* $\Phi' = TE(K_3, [i \;\; (3i+1)(i+1) \;\; 2(3i+1)(i+1)-1])$ *for* $i \in \mathbb{N}$. *Then* Φ *is cospectral to* Φ'.

Proposition 4.29. *Let* Φ *and* Φ' *be defined as* $\Phi = TE(K_3^*, [i(i+1)/2 \;\; i(i+1)/2+1 \;\; i(i+1)+1])$ *and* $\Phi' = TE(T_4, [1 \;\; i(i-1)/2 \;\; (i+1)(i+2)/2 \;\; i(i+1)])$ *for* $i \in \mathbb{N}$. *Then* Φ *is cospectral to* Φ'.

A single non-negative eigenvalue

Since the collection of signed digraphs that satisfy $\lambda_1 > 0 > \lambda_2$ on a given number of vertices is characterized by just two switching equivalence classes, we may use the structural information obtained in Section 4.4.1 to draw some quick conclusions with regard to their cospectrality.

Proposition 4.30. *Let* Φ *be either* K_n *or* K_n^*. *Then* Φ *is DES.*

Proof. Let D be cospectral to Φ. Then D has $\lambda_1 > 0 > \lambda_2$, and thus by Theorem 4.17, either $D \sim K_n$ or $D \sim K_n^*$. Suppose w.l.o.g. that $\Phi = K_n$ and $D \sim K_n^*$. Then, by Lemma 4.2 or 4.16, D is not cospectral to Φ, which is a contradiction. Thus, $D \sim \Phi$. □

Naturally, the same argument also holds when all edge gains are multiplied by -1.

Corollary 4.30.1. *Let* Φ *be either* $(K_n, -)$ *or* $(K_n^*, -)$. *Then* Φ *is DES.*

Smallest eigenvalue -1

A straightforward example to show that DES signed digraphs do not necessarily consist of a single connected component, possibly appended with a collection of disjoint vertices, carries over from graph theory.

Lemma 4.31. *Let* Φ *be an order-*n *connected signed digraph with* $\lambda_n = -1$. *Then* $\Phi \sim (K_n, +)$.

[8] Since their gains are a factor, the triangles in expansions of K_3 should all be counted twice.

Proof. Since Φ is connected, $\Gamma(\Phi)$ contains a shortest path $P_{u,v}$ for every $u, v \in V(\Phi)$. The result follows by two applications of interlacing: first to see that every such $P_{u,v}$ is length at most two, and thus $\Gamma(\Phi) = K_n$, and then to obtain that every induced triangle has gain 1. □

Proposition 4.32. *Let $m \in \mathbb{N}$ and $\Phi = \bigcup_{j=1}^{m}(K_{n_j}, +)$, $n_j \in \mathbb{N},\ j \in [m]$. Then Φ is DES.*

Proof. Note that Φ has smallest eigenvalue -1, and let D be cospectral to Φ. Then by Lemma 4.31, every connected component of D is switching isomorphic to a complete graph of appropriate order. The result follows since every positive eigenvalue characterizes such a connected component, and every zero eigenvalue corresponds to an isolated vertex. □

Corollary 4.32.1. *Let $m \in \mathbb{N}$ and $\Phi = \bigcup_{j=1}^{m}(K_{n_j}, -)$, $n_j \in \mathbb{N},\ j \in [m]$. Then Φ is DES.*

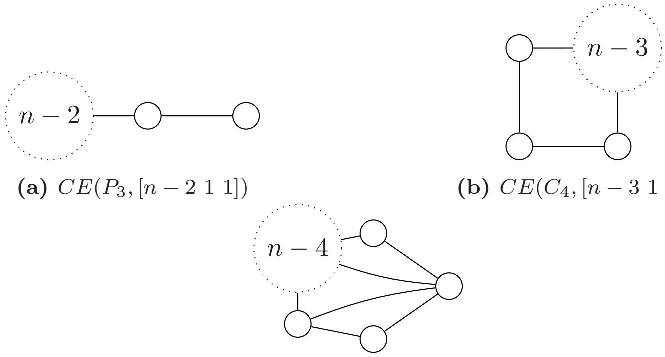
Weakly determined with $\lambda_2 > 0 > \lambda_3$

In the final section of this work, we will draw from the families of graphs characterized in Section 4.4, and use much of their inherent structure to obtain several more families of signed digraphs that are weakly determined by their $\mathcal{E}$-spectra.

In the below, we will use the same line of proof in two distinct situations, mainly separated by the numbers of edges and triangles that must (at least) occur in the corresponding underlying graphs. The considered graphs consistently contain relatively large cliques, which translate to a large number of triangles, relative to the contained number of edges. Implicitly, said graphs must also contain some vertices with substantially smaller degree, which is what will serve as the basis upon which the proofs are founded. Specifically, we will use the somewhat artificial notion of *edge-degrees*, formally defined as follows.

Definition 4.6. *Let $G = (V, E)$ be a graph and let $e = (u, v) \in E$ be an edge. If the vertex-degrees of u and v are respectively d_u and d_v, then the edge-degree $\delta(e)$ of e is $d_u + d_v$.*

The first infinite family of signed digraphs whose spectral characterization we will discuss is based on maximally dense clique expansions of C_4. Using the results from Section 4.2.2, we may be certain that any graph G that is underlying to a



(a) $CE(P_3, [n-2\ 1\ 1])$ **(b)** $CE(C_4, [n-3\ 1\ 1\ 1])$

(c) $CE(Gem, [1\ n-4\ 1\ 1\ 1])$

Figure 4.10 – The graphs in Lemma 4.33.

signed digraph D that is cospectral to such a clique expansion must contain precisely $\binom{n-1}{2}+1$ edges and at least $\binom{n-1}{3}-n+3$ triangles. Now, in case the minimum degree of G is small enough, we can easily use just the number of edges to pin-point its structure precisely, which is formalized in the following lemma.

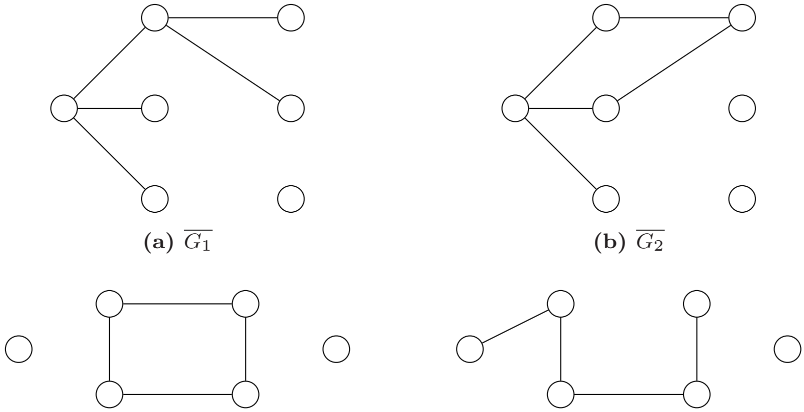
Lemma 4.33. *Let $n \geq 3$, and let G be an O_3-free graph with n vertices and $m = \binom{n-1}{2}+1$ edges. Futher, let u be the vertex of minimal degree. If $d_u = 1$, then $G \cong CE(P_3, [n-2\ 1\ 1])$. Moreover, if $d_u = 2$ then either $G \cong CE(C_4, [n-3\ 1\ 1\ 1])$ or $G \cong CE(Gem, [1\ n-4\ 1\ 1\ 1])$.*

If, instead, the minimum degree exceeds two, we may instead show that the graph must be one of four exceptional graphs on small n.

Lemma 4.34. *Let $n \geq 3$, and let G be an O_3-free graph with n vertices, $m = \binom{n-1}{2}+1$ edges and $t = |T(G)|$ triangles. Then $t \geq \binom{n-1}{3}-n+3$ if and only if G has minimum vertex degree 1 or 2, or if G is one of the exceptional graphs G_1, G_2, G_3, G_4, illustrated in Figure 4.11.*

Proof. First, we note that G cannot have an isolated vertex, because then the remaining $n-1$ vertices would have to harbour $\binom{n-1}{2}+1$ edges, which is impossible for a simple graph. Thus, suppose that every vertex has degree at least 3.

We will then consider the triangle-free complement $\overline{G} = (V, \overline{E})$ of G, whose degrees are denoted $d_u,\ u \in V$. This complement has $n-2$ edges, so $\sum_{u \in V} d_u = 2n-4$. By the above assumption, $d_u \leq n-4$ for $u \in V$.



(a) $\overline{G_1}$ (b) $\overline{G_2}$

(c) $\overline{G_3}$ (d) $\overline{G_4}$

Figure 4.11 – Complements of the four exceptional graphs for Lemma 4.34.

By inclusion-exclusion, we may express the number of triangles in G as

$$t = \binom{n}{3} - (n-2)^2 + \sum_{u \in V} \binom{d_u}{2}. \tag{4.4}$$

Here, the second term represents the $n-2$ edges missing from G, which are each responsible for $n-2$ missing triangles, unless they intersect with another missing edge. Then, using that $\overline{G}$ is K_3-free, the third term corrects the overshoot resulting from the second term.

Expanding the third term and plugging in $\sum_{u \in V} d_u$ and $\sum_{u \in V} d_u^2 = \sum_{e \in \overline{E}} \delta(e)$ yields

$$t = \binom{n}{3} - (n-1)(n-2) + \frac{1}{2} \sum_{e \in \overline{E}} \delta(e),$$

which may in turn be combined with $t \geq \binom{n-1}{3} - n + 3$ to find that

$$\sum_{e \in \overline{E}} \delta(e) \geq n^2 - 5n + 8.$$

Now, we may take the average of $\delta(e)$ over $\overline{E}$ to obtain

$$\frac{1}{n-2} \sum_{e \in \overline{E}} \delta(e) \geq n - 3 + \frac{2}{n-2} > n - 3. \tag{4.5}$$

So there is an edge e with $\delta(e) \geq n-2$. But $\delta(e) \leq n-1$, because $\overline{G}$ contains only $n-2$ edges. We distinguish two cases: either there is an edge with degree $n-1$, or there is not.

First, suppose that there is an edge $e^* = (u, v)$ with $\delta(e^*) = n-1$. Then $d_u = n-1-d_v$, and without loss of generality $d_v \leq d_u$. Now, since $\overline{G}$ is triangle-free and u and v are together adjacent to $n-3$ of the remaining vertices, the degree sequence of $\overline{G}$ is $n-1-d_v, d_v, 1, 1, \ldots, 1, 0$. Observe that since $d_u \leq n-4$, it follows that $3 \leq d_v \leq \frac{1}{2}(n-1)$, which we may use to we obtain an upper bound for $\sum_{e \in \overline{E}} \delta(e)$ as:

$$\sum_{e \in \overline{E}} \delta(e) = \sum_{w \in V} d_w^2 = d_v^2 + (n-d_v-1)^2 + (n-3) \leq 9 + (n-4)^2 + n - 3 = n^2 - 7n + 22.$$

Together with the lower bound $\sum_{e \in \overline{E}} \delta(e) \geq n^2 - 5n + 8$, this yields $n \leq 7$, which in turn implies $d_v = d_u = 3, n = 7$. This uniquely characterizes the graph G_1 since $\overline{G}$ is triangle-free and $\delta(e^*) = |E| + 1$.

Now, instead suppose that all edges have $\delta(e) \leq n-2$. As argued in (4.5), there is an edge $e^* = (u, v)$ with $\delta(e^*) = n-2$. This fixes all but one edge. Again, we have $d_u = n-2-d_v$, with $d_v \leq n-2-d_v \leq n-4$, so $2 \leq d_v \leq \frac{1}{2}n-1$. Working analogously to before, this case surprisingly yields the same upper bound for $\sum_{e \in \overline{E}} \delta(e)$:

$$\sum_{e \in \overline{E}} \delta(e) \leq d_v^2 + (n-2-d_v)^2 + 2 \cdot 4 + n - 6 \leq 4 + (n-4)^2 + n + 2 = n^2 - 7n + 22.$$

Because of the lower bound for $\sum_{e \in \overline{E}} \delta(e)$, we then find that $6 \leq n \leq 7$, and because $d_v \leq \frac{1}{2}n - 1$ that $d_v = 2$ and $d_u = n-4$. By checking the remaining 7 (non-isomorphic) configurations, if follows that G has sufficient triangles only when it is one of the remaining exceptional graphs G_2, G_3, or G_4. □

Given the above, we may now simply consider a limited number of potential underlying graphs and investigate in which cases they lead to cospectrality. Let C_4^* be the four-cycle with gain $-\omega$. Since it belongs to the only switching isomorphism class on C_4 that has eigenvalue -1 with multiplicity $n-3$, we may apply interlacing to conclude the following with relative ease.

Theorem 4.35. *Let $\Phi = CE(C_4^*, [n-3\ 1\ 1\ 1])$. Then Φ is DES, for $n \geq 4$.*

Proof. Suppose that D is cospectral to Φ. Then the spectrum of D contains 2 strictly positive and $n-2$ strictly negative eigenvalues; specifically, -1 occurs with multiplicity

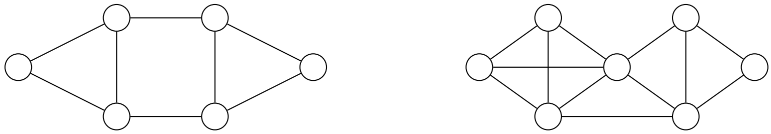
Figure 4.12 – A cospectral pair

$n-3$. Furthermore, $|E(D)| = \binom{n-1}{2} + 1$ and $|T(\Gamma(D))| \geq \binom{n-1}{3} - n + 3$, which by Lemma 4.34 implies that $\Gamma(D)$ contains a vertex of degree 1 or 2, or is one of four exceptional graphs. We first explore the four exceptions, illustrated in Figure 4.11.

Recall that graphs G_1, G_2, and G_4 contain exactly $|T(\Phi)|$ triangles, and thus $D = (G_j, \varphi)$, $j = 1, 2, 4$, may be cospectral to Φ only when all of its triangles (i.e., a basis of its cycle space) have gain 1. Using Proposition 4.4, it follows that D is switching isomorphic to its underlying graph. Then, simply computing the spectra of G_1, G_2, G_4 leads to the desired conclusion. If $D = (G_3, \varphi)$, then we find analogously that 6 triangles in D must have gain 1, and exactly two must have gain ω, which again leads to a unique switching isomorphism class on G_3, whose spectrum does not coincide with Φ. Thus, the exceptional cases are covered.

We move on to the general case: suppose $\Gamma(D)$ contains a vertex of degree at most 2. Then $\Gamma(D)$ is either $CE(P_3, [n-2\ 1\ 1])$, $CE(Gem, [1\ n-4\ 1\ 1\ 1])$ or $CE(C_4, [n-3\ 1\ 1\ 1])$, by Lemma 4.33. Now, it may easily be brute-forced that signed digraphs on *Gem* have at least 4 eigenvalues that are not -1. By an application of eigenvalue interlacing , it follows that signed digraphs on clique expansions of *Gem* have eigenvalue -1 with multiplicity at most $n-4$, which is insufficient. Similarly, signed digraphs on clique expansions of P_3 have eigenvalue -1 with multiplicity at most $n-3$; it is not hard to see that this is attained only when such a signed digraph is switching isomorphic to its underlying graph. Since $\operatorname{tr}(\mathcal{E})\,(CE(P_3, [n-2\ 1\ 1]))^3 > \operatorname{tr}(\mathcal{E})\,(\Phi)^3$, it follows that $\Gamma(D) = CE(C_4, [n-3\ 1\ 1\ 1])$. Finally, note that all triangles in D then must have gain 1, to satisfy $\operatorname{tr}(\mathcal{E})\,(D)^3 = \operatorname{tr}(\mathcal{E})\,(\Phi)^3$, and all of the 4-cycles must have gain $-\omega$, since C_4^* is the only 4-cycle with an eigenvalue -1. Since D coincides with Φ on all cycle gains, the conclusion follows by Proposition 4.3. □

Moreover, note that as a consequence of the proof above, we get the following for



(a) G_5 (b) G_6

Figure 4.13 – Exceptional graphs for Lemma 4.37

free, since all candidates for cospectrality that contain sufficient triangles are switching isomorphic.

Proposition 4.36. *$CE(P_3, [n-2\ 1\ 1])$ is DES for $n \geq 3$.*

At this point, the attentive reader may wonder whether the above holds analogously for clique expansions of the other switching classes on C_4. While most of the argument will hold up, we find that there are many signed digraphs on expansions of P_3 that have an eigenvalue -1 with sufficiently high multiplicity to potentially share the spectrum of such a C_4-expansion. In fact, an example of such a cospectral pair is shown in Figure 4.12. Thus, we would have to provide a substantially different approach; in the interest of unity, we move on to the next family of graphs.

In similar fashion, we may also consider maximally dense expansions of C_5, that satisfy $\lambda_2 > 0 > \lambda_3$. We follow largely the same line as in the proof of Lemma 4.34.

Lemma 4.37. *Let G be an O_3-free graph with $n \geq 5$ vertices, $m = \binom{n-2}{2} + 2$ edges and $t = |T(G)|$ triangles. Then $t \geq \binom{n-2}{3} - n + 4$ if and only if G is one of the following graphs:*

i) $CE(C_5, [n-4\ \ 1\ \ 1\ \ 1\ \ 1])$,

ii) $CE(P_4, [n-3\ \ 1\ \ 1\ \ 1])$, i.e., an $(n-2, 2)$-kite,

iii) $CE(P_4, [2\ \ 1\ \ n-4\ \ 1])$,

iv) One of the sporadic examples $CE(P_3, [3\ \ 1\ \ 3])$, G_5 or G_6. (See Figure 4.13.)

Proof. Like before, G cannot have an isolated vertex. If G has a vertex of degree 1, then the $n-2$ non-neighbors form a clique, and it follows that G is an $(n-2, 2)$-kite. For the remaining cases, we may assume that every vertex has degree at least 2.

Again consider $\overline{G}$, whose degrees are $d_u,\ u \in V$, and note that now $\sum_{u\in V} d_u = 4n-10$. Moreover, by assumption, $d_u \le n-3$ for $u \in V$. As before, by inclusion-exclusion, it follows that the number of triangles t in G may be expressed as

$$t = \binom{n}{3} - (2n-5)(n-2) + \sum_{u\in V}\binom{d_u}{2}.$$

Using that $\sum_{e\in\overline{E}} \delta(e) = \sum_{u\in V} d_u^2$ and the above, it follows that

$$t \ge \binom{n-2}{2} - n + 4 \iff \sum_{e\in\overline{E}} \delta(e) \ge 2n^2 - 8n + 10.$$

From this inequality, we will determine the several remaining options for $\overline{G}$. Once more, we take the average over $\overline{E}$ to see that

$$\frac{1}{2n-5}\sum_{e\in\overline{E}} \delta(e) \ge n - 2 + \frac{n}{2n-5} > n-2.$$

This implies that there is an edge $e^* \in \overline{E}$, such that $\delta(e^*) \ge n-1$. Note however that, because $\overline{G}$ is triangle-free, $\delta(e) \le n$. Now, either (I) there is an edge with degree n or (II) there is not.

(I): First, assume that $\overline{G}$ has an edge $e^* = (u,v) \in \overline{E}$ such that $\delta(e^*) = n$ and $d_u = n - d_v$. Without loss of generality, $d_v \le d_u$, and because $n - d_v \le n-3$, it follows that $3 \le d_v \le \frac{1}{2}n$.

Let $\overline{E}'$ be the set of $n-1$ edges in $\overline{E}$ that are incident to u or v, let $N_u = N(u)\setminus\{u,v\}$ be the set of neighbors of u besides v and similarly $N_v = N(v)\setminus\{u,v\}$. Because there are $n-4$ edges not in $\overline{E}'$, and because $\overline{G}$ is triangle-free, these are edges with one vertex in N_u and the other in N_v. Thus, $\sum_{w\in N_u}(d_w - 1) = \sum_{w\in N_v}(d_w-1) = n-4$. Now

$$\begin{aligned}\sum_{e\in\overline{E}'} \delta(e) &= \delta(e^*) + \sum_{w\in N_u}(d_w + n - d_v) + \sum_{w\in N_v}(d_w + d_v)\\ &= n^2 - (2d_v - 3)n + 2d_v^2 - 10.\end{aligned}$$

So for the remaining $n-4$ edges not in $\overline{E}'$ we require that $\sum_{e\notin\overline{E}'} \ge n^2 + (2d_v - 11)n - 2d_v^2 + 20$.

Suppose now that $d_v \ge 4$. Because the lower bound $n^2 + (2d_v - 11)n - 2d_v^2 + 20$

is the weakest for $d_v = 4$ (in the range $4 \leq d_v \leq \frac{n}{2}$), we obtain that

$$\sum_{e \notin \overline{E}'} \delta(e) \geq n^2 - 3n - 12, \text{ and thus } \frac{1}{n-4} \sum_{e \notin \overline{E}'} \delta(e) \geq n - 1 + \frac{2n-16}{n-4}.$$

This implies that the only possible values for n and d_v in this range is $n = 8$, $d_v = 4$, in which case $\delta(e) = n-1$ for all $e \in \overline{E}'$. It is easy to check however that this requires more edges than $\overline{E}'$ contains. In addition, it is easy to check that if $e \notin \overline{E}'$ then $\delta(e) \leq n-1$, for otherwise the complement of $\overline{E}'$ would consist of at least $n-3$ edges.

So instead we must have $d_v = 3$ and $\sum_{e \notin \overline{E}'} \delta(e) \geq n^2 - 5n + 2$. Averaging yields

$$\frac{1}{n-4} \sum_{e \notin \overline{E}'} \delta(e) \geq n - 2 + \frac{n-6}{n-4},$$

which implies that if $n > 6$ then there is an edge $\tilde{e} \notin \overline{E}'$ with $\delta(\tilde{e}) = n - 1$. Let us assume existence of $\tilde{e}$ for $n = 6$ as well, and let $\tilde{e} = (\tilde{u}, \tilde{v})$, with $\tilde{u} \in N_v$ and $\tilde{v} \in N_u$. Then there are two options. The first is that $\delta_{\tilde{v}} = 2$ and $\delta_{\tilde{u}} = n - 3$. This fixes all edges not in $\overline{E}'$, and we obtain the complement of $CE(P_4, [2\ \ 1\ \ n-4\ \ 1])$. The second option is that $d_{\tilde{v}} = 3$ and $d_{\tilde{u}} = n - 4$, where we may assume that $n > 6$, otherwise this is the same as the first option. Again, this fixes the entire graph. However only for $n = 7$ does it satisfy the requirements, and we obtain the complement of G_6. For $n = 6$, the above inequality does not guarantee the existence of an edge $\tilde{e} \notin \overline{E}'$ with $d(\tilde{e}) = n - 1$. Indeed, if we require all edges $e \notin \overline{E}'$ to have $\delta(e) \leq n - 2$, then we obtain the complement of G_5.

(II): Let us consider the possibility that, contrary to the case above, there is no edge $e \in \overline{E}$ with $\delta(e) = n$, but there is an edge $e^* = (u, v)$ such that $\delta(e^*) = n - 1$. Again, let $d_u = n - 1 - d_v$ and assume without loss of generality that $d_v \leq d_u$. Since $n - 1 - d_v \leq n - 3$, we now have that $2 \leq d_v \leq \frac{1}{2}(n-1)$. We proceed in the same way as before, but now $\overline{E}'$ has $n - 2$ edges. The main difference to (I) is that there is a vertex z that is not adjacent to u or v. That is: $V \setminus (N_u \cup N_v) = \{u, v, z\}$. In this case, we have that $\sum_{w \in N_u}(d_w - 1) + \sum_{w \in N_v}(d_w - 1) + d_z = 2(n-3)$ and therefore

$$\begin{aligned}\sum_{e \in \overline{E}'} \delta(e) &= n - 1 + (n - d_v - 2)(n - d_v - 1) + (d_v - 1)d_v + \sum_{w \in N_u} d_w + \sum_{w \in N_v} d_w \\ &= n^2 - (2d_v - 1)n + 2d_v^2 + 2d_v - 8 - d_z.\end{aligned}$$

It follows that for the remaining $n-3$ edges, we require

$$\sum_{e \notin \overline{E}'} \delta(e) \geq n^2 + (2d_v - 9)n - 2d_v^2 - 2d_v + 18 + d_z.$$

By averaging (as before) over the $n-3$ edges and using that this average is at most $n-1$, we find that we may restrict to the cases $d_v = 3$ with $7 \leq n \leq 9$ and $d_v = 2$ with $n \geq 5$. The latter case leads (as only possibility) to the complement of $CE(C_5, [n-4 \;\; 1 \;\; 1 \;\; 1 \;\; 1])$.

For $d_v = 3$, we have $\sum_{e \notin \overline{E}'} \delta(e) \geq n^2 - 3n - 6 + d_z$ and $d_w \leq n-4$ for all $w \in V \setminus \{z\}$. If $d_z \geq 1$, then consider an edge e' incident to z. It must satisfy $\delta(e') \leq d_z + n - 4$, and thus

$$\sum_{e \notin E' \cup \{e'\}} \delta(e) \geq n^2 - 4n - 2.$$

But then $\frac{1}{n-4} \sum_{e \notin E' \cup \{e'\}} \delta(e) \geq n-1$, which is a contradiction.

Therefore, $d_z = 0$, and we have to add $n-3$ edges between N_u and N_v. For $n=7$, this yields $K_1 \cup K_{3,3}$, which is the complement of our final sporadic example $CE(P_3, [3 \;\; 1 \;\; 3])$. For $n = 8, 9$, it is easily verified that the corresponding graphs (respectively the complements of $K_1 \cup K_{3,4}$ minus one edge, and $K_1 \cup K_{3,5}$ minus two edges) contain insufficient triangles, which concludes the proof. □

Theorem 4.38. *Let $G = CE(C_5, \tau)$ with $\tau = [n-4 \;\; 1 \;\; 1 \;\; 1 \;\; 1]$, and let $\Phi = (G, \varphi)$ where φ is of type A or C. Then Φ is DES.*

Proof. Suppose that D is cospectral to Φ. Using Lemma 4.2, it follows that $\Gamma(D)$ contains at least $\frac{1}{6}\mathrm{tr}\,(\mathcal{E})\,(\Phi)^3 = \binom{n-2}{3} - n + 4$ triangles, which by Lemma 4.37 implies that $\Gamma(D)$ is one of at most six potential graphs. Analogously to the proof of Theorem 4.35, it may easily be evaluated that the sporadic cases are not underlying to any signed digraphs that are cospectral to appropriately sized Φ, so we focus on the general case.

Suppose that $\Gamma(D) = CE(P_4, [n-3 \;\; 1 \;\; 1 \;\; 1])$; an $(n-2, 2)$-kite. By Corollary 4.21.1, the signed digraph that is induced by the $(n-2)$-clique is switching isomorphic to K_{n-2} or K_{n-2}^*. This implies that $\frac{1}{6}\mathrm{tr}\,(\mathcal{E})\,(D)^3 \geq \binom{n-2}{3} - \frac{1}{2}(n-4) > \frac{1}{6}\mathrm{tr}\,(\mathcal{E})\,(\Phi)^3$, which is a contradiction.

Next, suppose that $\Gamma(D) = CE(P_4, [2 \;\; 1 \;\; n-4 \;\; 1])$. Then $\Gamma(D)$ contains exactly one more triangle than G for every $n \geq 5$, which implies that $\mathrm{tr}\,(\mathcal{E})\,(D)^3 \neq \mathrm{tr}\,(\mathcal{E})\,(\Phi)^3$, and we again obtain a contradiction. Hence, $\Gamma(D) = CE(C_5, [n-4\ \ 1\ \ 1\ \ 1\ \ 1])$, and the conclusion regarding φ follows by Proposition 4.3. $\square$

As before, we can draw similar conclusions for other graphs considered above.

Theorem 4.39. *Let G be an $(n-2,2)$-kite, $n \geq 3$, and let $\Phi = (G, \varphi)$ be such that the induced $(n-2)$-clique is switching isomorphic to either K_{n-2} or K^*_{n-2}. Then Φ is DES.*

Proof. By Corollary 4.21.1, Φ has $\lambda_2 > 0 > \lambda_3$, so Lemma 4.37 is applicable if $n \geq 5$. Now, observe that for $n > 6$, $\frac{1}{6}\mathrm{tr}\,(\mathcal{E})\,(\Phi) > \binom{n-2}{3} - n + 5$, which is the largest number of triangles in any graph in Lemma 4.37 that is not itself an $(n-2,2)$-kite. The conclusion follows easily by brute-forcing (by computer) the limited collection of signed digraphs from Lemma 4.37 on $n = 4, 5, 6$ whose underlying graphs do contain sufficient triangles. (Recall that if $n = 3$ then $\Phi \sim G$, by Proposition 4.4.) $\square$

Finally, as an immediate consequence of Theorems 4.38 and 4.39, the following is easily verified. Since all cospectral candidates for $n \geq 8$ are DES themselves, one only needs to check a limited number of graphs on $5 \leq n \leq 7$.

Proposition 4.40. *$CE(P_4, [2\ 1\ n-4\ 1])$ is DES.*

To conclude, we note that there are various families of signed digraphs that are close tangents of the discussed DES families, which have remained untreated in this section. For example, maximally dense C_5 expansions with signatures B and D, or minimally connected semi-complete graphs come to mind. While the author is convinced that similar results could be obtained for these cases, their particular challenges are preserved for future research.

4.6 Open questions

We end this chapter with a summarizing list of open questions.

Question 4.1. *For a given underlying graph, there is a switching equivalence class whose edges have gain 1 on a predetermined spanning tree. However, is it possible to determine (or bound) the number of members of said class that do so?*

Question 4.2. *An interesting, 'ugly' example of a signed digraph whose spectrum is symmetric was provided in Figure 6.2. Perhaps, it is too ambitious to ask for a tight characterization of all signed digraphs with symmetric spectra. However, would it be possible to formulate some necessary properties?*

Question 4.3. *The collections of signed digraphs whose rank is either* 2 *or* 3 *have been completely characterized. Do ranks* 4 *and up also allow for a comprehensive characterization?*

Question 4.4. *In order to keep the discussion on signed digraphs with two non-negative eigenvalues tidy, we have zoomed in on a number of special cases. Is it feasible to complete the characterization? Possibly under some additional restrictions?*

Question 4.5. *How do the results of this work change when one considers other gain groups $\mathbb{T}_k$? Which parts carry over to a gain set that is not closed under multiplication?*

Question 4.6. *Do the remaining columns of Table 4.2 give rise to DES signed digraphs? And what about other signed digraphs on C_4?*

Question 4.7. *In our representation, $\varphi(u, v)$ is positive if and only if $\varphi(v, u)$ is positive. In dynamical systems, this does not have to be the case. Should we adapt our formulation to accommodate for these 'negative feedback loops', or can the issue be sufficiently circumvented with a simple subdivision trick? Moreover, can spectral analysis of $\mathbb{T}_6$-gain graphs then offer new insights into the (possible) stability of such systems?*

CHAPTER 5

Computer-aided search for gain graphs with predetermined properties by Simulated Annealing

Abstract

A common first step in any classification of graphs would be to employ the help of a computer. Classically, a simple exhaustive search on graphs of small order would suffice. However, this approach quite quickly fails if one is looking for gain graphs, as a consequence of their continuous nature. As a surprisingly effective solution to this issue, we apply a technique from continuous optimization called *Simulated Annealing* to obtain gain graphs whose eigenvalues satisfy a predetermined property.

5.1 Introduction

A natural way to start off an investigation into graphs of any sort that are united in satisfying some sort of property is to work off of a collection of satisfactory examples, in order to test initial hypotheses. While such examples will often be more or less readily available in the literature, it is quite common to apply some sort of search. In traditional graph related fields, one is often inclined to iteratively consider all graphs within a given band of parameters. While this may be somewhat time consuming, one at least has the guarantee that all possible examples of graphs with the desired property, in the domain of the search, are found.

However, if one is interested in complex unit gain graphs; effectively weighted graphs with weights on the complex unit circle, such an approach does not work. Indeed, observe that by their continuous nature, considering "all" gain graphs of a given order is simply impossible. One may turn this weakness into a strength by observing that the shift to a continuous paradigm opens the door to various highly effective continuous optimization procedures. For example, one might minimize the summed quadratic distances of the (ordered) eigenvalues of a gain graph Ψ to a predetermined choice of spectrum, by treating the edge gains as variables. While failure to find a candidate does not conclusively prove that none exists, one can certainly use the output of such a search when said sum total is close to zero.

Below, we describe the applied method, a well-known procedure known as *simulated annealing*. We conclude the chapter with a brief discussion on performance observations and potential applications.

5.2 Simulated annealing

To overcome some of the challenges presented by the gain graph paradigm, we have implemented a search method that is somewhat unusual in this context, though generally well-known. Specifically, a Simulated Annealing [69] algorithm, which is commonly found in more applied optimization applications, has turned out to fit our needs. Some recent, particularly successful applications of this process in various applied fields include [34, 79, 94, 113].

Briefly put, the procedure searches randomly around some 'currently best candidate,' moving to a new candidate with probability 1 if it is 'better' and with some probability smaller than 1 if it is 'worse.' The latter probability is dependent on the relative qualities of the old and the new candidates. Moreover, the variability (i.e., how 'different' a new candidate is from the old candidate) gradually changes over time, such that the algorithm starts off exploring the possibilities somewhat overzealously, and then cautiously exploiting the current best solution before terminating the search.

More than anything, the evaluation of the quality of a candidate is crucial to the success of the method. This is usually done with some function $f(\cdot)$. The evaluation should be continuous in the sense that movement in the 'right direction' is correctly captured. To state the obvious: the evaluation function

$$g(A) = \begin{cases} 0 & \text{if } A \text{ satisfies the desired property} \\ 1 & \text{otherwise,} \end{cases}$$

will not be of any use, as it will not be able to distinguish between candidates that are 'close' or not. If one is interested in finding gain graphs whose spectrum consists of the (ordered) eigenvalues $\mu_1, \ldots, \mu_n$, a simple quadratic distance metric appears to work well. That is,

$$f(A) = \sum_{j=1}^{n} (\lambda_j - \mu_j)^2, \tag{5.1}$$

where the λ_j are the eigenvalues of A. For different applications, other evaluation functions may be desirable. These may be slight alterations of (5.1), such as

$$f(A) = \sum_{j=1}^{n} (\lambda_j + \lambda_{n-j+1})^2, \tag{5.2}$$

which is used in Chapter 6, in order to gain a foothold for the proposed discussion concerning gain graphs with symmetric spectra. Alternatively, some instances might require a more tailored fit.

In Chapter 7, we will be looking for gain graphs with exactly two distinct eigenvalues. Any gain matrix A that satisfies this requirement admits to the equation $A^2 - aA + kI = O$. Taking the norm of the left-hand side would in some sense measure how far A is removed from satisfying this equality. Thus, we use the evaluation function

$$f(A) = \|A^2 - (\lambda_1 + \lambda_n)A + \lambda_1\lambda_n I\|, \tag{5.3}$$

where λ_1 and λ_n are respectively the largest and the smallest eigenvalues of A.

We have found it most convenient to fix the underlying graph to some input value, and to only allow the gains of the edges to vary. In particular, since said gains are all in $\mathbb{T}$, one may simply rotate the gain values around the complex unit circle with a random amount to move from on candidate to the next in a rather controllable fashion. Broadly speaking, the procedure for a given input graph may then be described as follows.

Algorithm 5.1 Gain graph search by Simulated Annealing *(sketch)*

Input: Cool-down parameter $0 < \alpha < 1$; Initial temperature $0 < t \leq 1$; minimum temperature $\tau > 0$; terminal value ε (small); iterations m bidirected graph G; evaluation function $f(\cdot)$
Output: Gain graph Ψ, Valuation v

```
Initialize
Set old ← G
Fix a spanning tree of the edges of old; randomly assign the other edges a gain.

while t > τ do
    for j = 1, ..., m do
        Set new ← old

        Randomly mutate the new candidate
        For each non-fixed edge (u, v) in new do
            Randomly draw r from U(−1, 1)
            Set ψ_new(uv) ← exp(iπ · r · t) · ψ_old(uv) and ψ(vu)_new ← ψ_new(uv)^(−1).
        Compute f(old) and f(new).

        Terminate if target is met, or choose from which candidate to continue
        if f(new) < ε then
            Set Ψ ← new and v ← f(new), return
        else
            Set p ← min {exp ((f(old) − f(new))/(f(old) · t)) , 1} .
            Randomly draw r from U(0, 1)
            if r ≤ p then
                Set old ← new
    Set t ← ατ
Set Ψ ← old, v ← f(old), return.
```

Here, the initialization step uses the fact that a more general version of Proposition 4.4 holds for general gain graphs. Even when the value of the function f is reasonably low, at the end of the procedure above, it yields gain graphs which only *approximately* satisfies the desired property; one still has to distill the actual exact gain graph, to which the procedure had been converging.

5.3 Performance

Simulated Annealing, in general, satisfies some very strong theoretical convergence results [62]. Loosely put: if (I) the search neighborhoods are sufficiently connected[1] and (II) the cool-down is sufficiently slow, then there are probabilistic guarantees that the global optimum is found. The former condition is true, for Algorithm 5.1, but the latter is less black-and-white.

In particular, since one might be searching for something that does not necessarily exist for the selected underlying graph, one has to make a trade-off between speed and accuracy. If one decides on a quicker cool-down procedure (that is, higher α and/or lower m), Algorithm 5.1 may not converge to an output that globally minimizes f. This translates to not finding an example with the desired property, while there would have been one to find.

To showcase this trade-off, we have tested the success rate of this procedure by searching for two-eigenvalue gain graphs on the underlying graphs of various known two-eigenvalue gain graphs Ψ of increasing order and density. Specifically, we (through trial and error) settled on two distinct set-ups, which are outlined by Table 5.1. We primarily tune with *initial temperature*, *iterations per temperature* (m) and the *cool-down procedure*, though they all more or less accomplish the same thing: more iterations of the random search, at some point in the temperature curve. The former (speed) one that has terminated each call in under 10 seconds and the latter (accuracy) that successfully found an example at least 95% of its calls. Their respective success rates and computation times, for various underlying graphs, are shown in Figure 5.1. With the exception of the complete graphs, that somehow converge remarkably well in the quick set-up, we observe a clear trade-off.

As one might expect, the main challenge (particularly when the considered graphs become relatively dense) is getting sufficiently close to the true example in the final stages of the search. This ties seamlessly with one of the drawbacks of the proposed procedure: even when the output matrix A is very close to a gain graph with the desired property, e.g. $f(A) = 0.02$, it is still not a trivial matter to arrive at the

[1] In the sense that any candidate may be mutated a (possibly huge) number of times to become any one other candidate, for our case.

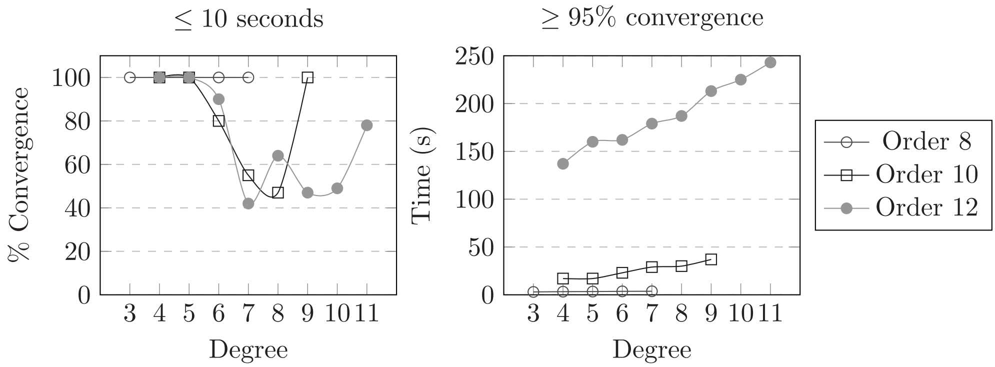


Figure 5.1 – Statistics on simulated annealing calls on admissible underlying graphs that converge to a gain graph with two eigenvalues. (40 calls for each admissible graph.)

	Speed	Accuracy
α	0.98	0.995
t	0.2	0.2
τ	0.001	0.001
m	50	400
ε	0.0001	0.0001

Table 5.1 – Tuning parameters corresponding to Figure 5.1

true gain graph. Refinement of this final step could go a long way to improving the applicability of this procedure.

Additionally, while it has served our needs just fine, the current implementation is still relatively crude. The expansive body of research on the subject of simulated annealing contains many potential modifications (see, e.g., [34]) that might further improve the search method itself. Moreover, it seems likely that performance can be significantly improved with more dedicated research and optimization; as it stands, methods in this chapter have played a mostly supporting role.

5.4 A selection of the results

In the interest of completeness, we include some of the results that have been found using the methods described in this chapter, which do not appear elsewhere in this work.

5.4.1 Signed digraphs

The described simulated annealing procedure has been applied to find a number of signed directed graphs with exactly two non-negative eigenvalues. In order to ensure that the results would be $\mathbb{T}_6$-gain graphs, we added what may effectively be considered a penalty component[2]

$$p(A) = c \cdot \sum_{(u,v)\in E} \|A_{uv} - \mathcal{E}_{uv}\|^2, \tag{5.4}$$

where $\mathcal{E}_{uv} = \arg\min_{x\in\mathbb{T}_6} \|A_{uv} - x\|$ and $c = 5$, to the evaluation function f.

Various evaluation functions could theoretically work here; one could simply minimize λ_3. (Note that λ_2 may easily be shown to be necessarily non-negative, except when the underlying graph is complete.) However, we found that minimizing the somewhat arbitrary-looking evaluation function

$$f(A, \lambda_1, \ldots, \lambda_n) = (\lambda_3 + 1)^2 + (\lambda_4 + 1)^2 + (\lambda_5 + 1)^2 + p(A) \tag{5.5}$$

worked relatively well.

Application of the described search procedure on random underlying graphs (being mindful to ensure that said underlying graphs contain no order-3 stable sets), we find various examples on underlying graphs that are not (although they do contain) clique expansions of C_5 or P_4. As an interesting aside, repeated runs of the search on underlying graphs that we know to admit a signed digraph with exactly two non-negative eigenvalues are almost always equally successful. Some of the obtained graphs are included, below.

[2] In hindsight, it might have made more sense to apply a discrete version of SA. That is, rather than rotating the non-fixed gains a random distance that decreases over time, instead only allow the sixth roots of unity and rotate with decreasing (w.r.t. time as well as distance) probability. As a proof of concept, this has been implemented and found to work more quickly than the penalty-based method, though no extensive studies were done using this alternative.

$$\mathcal{E}_1 = \begin{bmatrix} 0 & 0 & 0 & \bar{\omega} & 1 & 1 & 1 & \bar{\omega} & \bar{\omega} & 1 \\ 0 & 0 & -1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & -1 & 0 & 0 & -\bar{\omega} & 0 & 0 & 0 & 0 & 1 \\ \omega & 1 & 0 & 0 & -\bar{\omega} & \omega & \omega & 1 & 1 & 1 \\ 1 & 0 & -\omega & -\omega & 0 & 1 & 1 & -\omega & -\omega & 1 \\ 1 & 0 & 0 & \bar{\omega} & 1 & 0 & 1 & \bar{\omega} & \bar{\omega} & 1 \\ 1 & 0 & 0 & \bar{\omega} & 1 & 1 & 0 & \bar{\omega} & \bar{\omega} & 1 \\ \omega & 1 & 0 & 1 & -\bar{\omega} & \omega & \omega & 0 & 1 & 1 \\ \omega & 1 & 0 & 1 & -\bar{\omega} & \omega & \omega & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}, \quad \lambda_3 = -0.1575.$$

$$\mathcal{E}_2 = \begin{bmatrix} 0 & -\bar{\omega} & \bar{\omega} & 0 & 1 & 1 & 1 & 0 & 1 & \omega \\ -\omega & 0 & 0 & \omega & 1 & -\omega & -1 & 0 & -1 & \bar{\omega} \\ \omega & 0 & 0 & 0 & 1 & \omega & \omega & -\omega & \omega & \omega \\ 0 & \bar{\omega} & 0 & 0 & 1 & 0 & 0 & \omega & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & -\bar{\omega} & \bar{\omega} & 0 & 1 & 0 & 1 & 0 & 1 & \omega \\ 1 & -1 & \bar{\omega} & 0 & 1 & 1 & 0 & -\bar{\omega} & 1 & \omega \\ 0 & 0 & -\bar{\omega} & \bar{\omega} & 1 & 0 & -\omega & 0 & -\omega & 0 \\ 1 & -1 & \bar{\omega} & 0 & 1 & 1 & 1 & -\bar{\omega} & 0 & \omega \\ \bar{\omega} & \omega & \bar{\omega} & 1 & 1 & \bar{\omega} & \bar{\omega} & 0 & \bar{\omega} & 0 \end{bmatrix}, \quad \lambda_3 = -0.2080.$$

$$\mathcal{E}_3 = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & -\bar{\omega} & 0 & 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & 0 & \omega & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & -\bar{\omega} & 0 & \omega & 0 & 0 & -1 & 0 & 1 & 1 \\ 0 & \bar{\omega} & -\omega & 0 & 1 & \omega & 1 & \bar{\omega} & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ -\omega & 1 & \bar{\omega} & \bar{\omega} & 0 & 0 & 0 & 0 & -\bar{\omega} & 0 & -\omega & -\omega \\ 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & \omega & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ -1 & 0 & -1 & 0 & 0 & -\omega & 0 & 1 & 0 & 0 & -1 & -1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & -\bar{\omega} & 0 & 0 & -1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & -\bar{\omega} & 0 & 0 & -1 & 0 & 1 & 0 \end{bmatrix}, \quad \lambda_3 = -0.0757.$$

$$\mathcal{E}_4 = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & \bar{\omega} & \omega & 1 & 1 & 0 & 1 & -\omega & 0 \\ 0 & 0 & 0 & \omega & 0 & \omega & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & \bar{\omega} & \bar{\omega} & 0 & \bar{\omega} & \bar{\omega} & 0 & \bar{\omega} & \bar{\omega} & 0 \\ 0 & 0 & 0 & 1 & 1 & \omega & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & \omega & 1 & 0 & 0 & 1 & \bar{\omega} & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & \omega & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & -\bar{\omega} & 0 & \omega & 1 & \omega & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \end{bmatrix}, \quad \lambda_3 = -0.004.$$

5.4.2 Symmetric spectra

During the initial exploration for the material that will be discussed in Chapter 6, we found that gain graphs with symmetric spectra seem to be relatively common, in the sense that many switching-distinct examples were found on the same underlying graphs. To illustrate the degree to which this held up, we present a repeated search for gain graphs with symmetric spectra on 500 random underlying graphs of orders $n = 20, 40, 60, 80$ with evaluation function

$$f(\lambda_1, \dots, \lambda_n) = \sum_{j=1}^{n} (\lambda_j - \lambda_{n-j+1})^2. \tag{5.6}$$

For each underlying graph, the search is performed 50 times; the results are shown in Table 5.2. Not only does the algorithm consistently finds a candidate in each run, we also observe that the outputs corresponding to the same underlying graph are all pairwise switching-distinct (in fact, pairwise not cospectral). This lead us to believe the somewhat surprising suspicion that the statement “almost every graph is underlying to infinitely many switching distinct gain graphs with symmetric spectra,” which is discussed in detail in Chapter 6, could possibly be true. As an aside, note that the terminal values increase in a roughly linear fashion, which corresponds to linearly increasing number of quadratic differences that are summed.

n	Total calls	# Switching classes	max $fval$ $(\times 10^{-4})$
20	25000	25000	2.3
40	25000	25000	6.4
60	25000	25000	11.1
80	25000	25000	15.5

Table 5.2 – Repeated search for gain graph with symmetric spectra on 500 random underlying graphs Γ; 50 calls for each Γ.

5.4.3 Two-eigenvalue gain graphs

Finally, the procedure has been applied to obtain gain graphs with precisely two distinct eigenvalues, for Chapter 7. Most notably, a systematic search of two-eigenvalue gain graphs on order-12, degree-5 graphs, we found precisely $M_1, \ldots, M_4$, shown in Examples 5.3-5.5, in addition to the order-12 donut (see Section 7.6.4). As mentioned before, we cannot be absolutely certain that no other examples exist due to the random nature of the search algorithm, but the author is reasonably confident that all two-eigenvalue gain graphs with $(n, k) = (12, 5)$ have been found.

We include a list of new examples, which will not appear in Chapter 7. Other candidates, such as the one presented in Example 7.1, have also been obtained via the described search procedure, though they turned out to have appeared elsewhere, first.

Example 5.1. *New example on K_8:*

$$K_8^* = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & i & -i & i & -i & i & -i \\ 1 & -i & 0 & -i & -i & i & i & i \\ 1 & i & i & 0 & -i & -i & -i & i \\ 1 & -i & i & i & 0 & i & -i & -i \\ 1 & i & -i & i & -i & 0 & i & -i \\ 1 & -i & -i & i & i & -i & 0 & i \\ 1 & i & -i & -i & i & i & -i & 0 \end{bmatrix}.$$

Example 5.2. *A signed graph example on K_{10}:*

$$K_{10}^* = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 0 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 0 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 0 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & 0 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & 1 & 1 & 0 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & 0 & 1 & -1 \\ 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 0 & -1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & 0 \end{bmatrix}.$$

Example 5.3. *New example on the icosahedron:*

$$M_1 = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & -1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & -1 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & -1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & x & 0 & 0 & 0 & -1 & -1 & -x \\ 1 & 0 & 0 & 0 & \bar{x} & 0 & -1 & 0 & 0 & 0 & -\bar{x} & 1 \\ 1 & 1 & 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & -1 \\ 1 & -1 & -1 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & -1 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & -1 & 0 & 0 & 0 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 & -x & 0 & 0 & 0 & -1 & 0 & x \\ 1 & 0 & 0 & 0 & -\bar{x} & 1 & -1 & 0 & 0 & 0 & \bar{x} & 0 \end{bmatrix}, \; x \in \mathbb{T}.$$

Example 5.4. *A bipartite example based on a new non-graphical weighing matrix of* *weight 5:*

$$Z = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & -\bar{x} & -1 & \bar{x} & 0 & -x \\ 1 & -1 & x & 0 & -x & x \\ 1 & \bar{x} & 0 & -\bar{x} & -1 & -x \\ 1 & 0 & -x & -1 & x & x \\ 0 & \bar{x} & -\bar{x} & \bar{x} & -\bar{x} & 1 \end{bmatrix}, x \in \mathbb{T}, \textit{ and } M_2 = \begin{bmatrix} O & Z \\ Z^* & O \end{bmatrix}.$$

Example 5.5. *Two more sporadic examples:*

$$M_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & -x & x & x & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & x & -x & 0 & -x \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -x & x \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & -1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & -1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & x & -x \\ 1 & 0 & -\bar{x} & \bar{x} & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & \bar{x} & -\bar{x} & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & \bar{x} & 0 & -\bar{x} & 0 & 0 & \bar{x} & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & -\bar{x} & \bar{x} & 0 & 0 & -\bar{x} & 0 & 0 & 0 & 0 \end{bmatrix}, x \in \mathbb{T}, \textit{ and}$$

$$M_4 = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & 0 & 0 & -1 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 & i & 0 & -i & -i & i & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & -i & i & -i & 0 & i \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & i & i & -i & 0 & -i \\ 1 & 1 & 1 & -i & 0 & 0 & 0 & 0 & 0 & i & 0 & 0 \\ 0 & 1 & -1 & 0 & i & -i & 0 & 0 & 0 & 0 & 0 & -i \\ 1 & 0 & 0 & i & -i & -i & 0 & 0 & 0 & 0 & -i & 0 \\ 1 & 0 & 0 & i & i & i & -i & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & -i & 0 & 0 & 0 & 0 & i & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & -i & i & 0 & i & 0 & 0 & 0 & 0 \end{bmatrix}.$$

5.5 Potential other applications

Since the backbone of the described search method is essentially independent of what we have been searching for in the context of this particular project, it should be noted that such search procedures could potentially be extremely useful in similar contexts. The search primarily hinges on the evaluation function f and the idea that one could move "gradually closer" to satisfying the desired property, and as such seems to work well for various spectral properties of gain graphs.

Another interesting avenue to explore could be to turn ones attention to the search for, e.g., new strongly regular graphs, or new distance regular graphs. Such searches could be performed indirectly, by instead searching for equivalent gain graphs (see, for example, [24, 66, 37]) or one could theoretically also move away from the fixed underlying graphs. The most important issue to tackle in order for the latter searches to be fruitful, would be to come up with a reasonable evaluation criterion. In particular, one would need to find a way to deal with the discrete nature of a graph, compared to the continuous nature of the gains, which might be challenging. Nevertheless, it might be interesting to try something unusual in a field that has come up with very few new examples over the past two decades.

CHAPTER 6

Symmetry in complex unit gain graphs and their spectra

Abstract

Complex unit gain graphs may exhibit various kinds of symmetry. In this chapter, we explore structural symmetry, spectral symmetry and sign-symmetry in gain graphs, and their respective relations to one-another. Our main result is a construction that transforms an arbitrary gain graph into infinitely many switching-distinct gain graphs whose spectral symmetry does not imply sign-symmetry. This effectively provides a much more general answer to the gain graph analogue to an existence question that was recently treated in the context of signed graphs.

6.1 Introduction

Throughout the natural sciences, symmetry might be the single most widely recognized feature that is in some way beautiful, useful, or both. It, therefore, occurs in various forms. Of particular interest to the author is symmetry in the eigenvalues of graphs and their diverse generalizations. A collection of eigenvalues (also called the *spectrum*) is said to be symmetric if it is invariant under multiplication by -1. Two recent works that consider symmetry in eigenvalues are [56, 48].

In addition to spectral symmetry, two more instances of symmetry come up in this work. Likely the best known of the two is concerned with the existence of multiple assignments of the same collection of labels to graph vertices, that cannot be distinguished by looking at the adjacency and non-adjacency of pairs of vertices. That is, a graph is said to be (structurally) symmetric if it has any non-trivial automorphism. Structurally, this (asymptotically rare) property implies that parts of the graph are akin to one-another, as well as identical in relation to their mutual complement.

Finally, we encounter a phenomenon known as sign-symmetry. A particular line of research is concerned with the invariance of signed graphs, which was introduced some time ago by Zaslavsky [109], under negation of their sign functions. In particular, if (G, σ) is switching isomorphic (see Def. 1.7) to $(G, -\sigma)$, it is said to be sign-symmetric. Its relation to spectral symmetry is interesting: while sign-symmetry implies a symmetric spectrum, the reverse relation fails, in general. Sporadic examples of signed graphs that show the latter phenomenon on complete graphs, as well as various such infinite families have been found by Ghorbani et al. [42].

In the current article, we consider these types of symmetry, and the relation between them, in the complex unit gain graph paradigm. These objects are, effectively, weighted bidirected graphs with weights on the complex unit circle, such that the weight of every arc is equal to the inverse weight of its converse arc. In a recent (re)popularization, the generalizations of various well-studied graph theoretical objects, such as signed graphs and the Hermitian adjacency matrices for directed graphs [51, 76, 84], have seen quite some attention. Applications of gain graphs are primarily related to quantum state transfer [23], and spectral analysis of these objects has yielded a number of interesting parallels to complex geometry, such as those discussed in Chapter 7.

While some relations between the aforementioned symmetries are clear, the existence of (an infinite family of) signed graphs which are spectrally symmetric but not sign-symmetric was open until recently, when Ghorbani et al. [42] constructed the

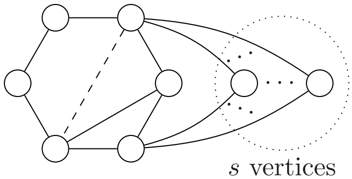


Figure 6.1 – The signed graph Γ_s. Here, the dashed edge has gain -1.

family Γ_s (illustrated in Figure 6.1) and proved that such signed graphs exist. While mention is made of other infinite families that have the desired property, they seem to effectively involve adding vertices to the leftmost hexagon in Figure 6.1. Thus, this article addresses a natural follow-up question, and asks what happens when the framework is generalized to encompass all complex unit gain graphs, rather than just signed graphs.

As a gentle introduction to the subject matter, we first consider spectral symmetry of gain graphs. We show that a graph G is underlying to only spectrally symmetric gain graphs if and only if it is bipartite, and that every graph is underlying to some spectrally symmetric gain graphs. Then, we consider a number of doubling operations whose origin lies with a well-known recursive construction of Hadamard matrices. By design, these constructions yield gain graphs with symmetric spectra. While most of them also implicitly yield sign-symmetric gain graphs, we prove that a subtle adaptation of Sylvester's double transforms an arbitrary gain graph into infinitely many switching-distinct gain graphs that are not sign-symmetric.

The contents of this paper are organized as follows. First, we provide a thorough introduction of all of the concepts used in this article. This is followed by a discussion of various constructions of gain graphs with symmetric spectra, in Section 6.3. While most of these constructions are sign-symmetric by design, we prove that an appropriate adaptation of Sylvester's double, in general, is not. To conclude this article, Section 6.5 puts a spotlight on an open question concerning the general (asymptotic) case. Specifically, we have come to believe that the vast majority of graphs is underlying to an infinite number of switching-distinct gain graphs that is spectrally symmetric but not sign-symmetric.

6.2 Preliminaries

We recall some of the essential definitions specific to this chapter, which concerns various kinds of symmetry in complex unit gain graphs. A graph G is said to be symmetric if it has a non-trivial automorphism.

If a gain graph is such that it has an eigenvalue λ with multiplicity m only if it also has an eigenvalue $-\lambda$ with multiplicity m, then it is said to have a *symmetric spectrum* or be *spectrally symmetric.* The following is a well-known property of diagonalizable matrices.

Lemma 6.1. *Let Ψ be a unit gain graph with underlying graph G and characteristic polynomial $\chi(\lambda)$ as in* (1.1)*. Then Ψ has a symmetric spectrum if and only if $a_j = 0$ for all odd $j \leq n$.*

We say that a graph G *allows symmetric gain-spectra* if there exists a gain graph Ψ on G whose spectrum is symmetric; if moreover all gain graphs on G have symmetric spectra then we say that G *requires* symmetric gain-spectra.

The *negation* of a gain graph Ψ is found by multiplying the gain of every arc with -1. This is commonly simply denoted as $-\Psi := (G, -\psi))$. A gain graph is said to be *sign-symmetric* if it is switching isomorphic to its negation; that is, if $\Psi \sim -\Psi$.

A useful concequence of Propositon 4.3 is the following.

Lemma 6.2. *Let Ψ be a gain graph, and let $\gamma_k(\mu)$ denote the number of distinct order-k cycles in Ψ with $Re(\phi(C)) = \mu$. If it holds that $\gamma_{2k-1}(\mu) \neq \gamma_{2k-1}(-\mu)$ for some $\mu \in \mathbb{R}$ and $k \in \mathbb{N}$, then Ψ is not sign-symmetric.*

6.2.1 Initial observations

We briefly discuss the more obvious relations between the different notions of symmetry. Firstly, neither one of spectral symmetry and structural symmetry implies the other. For the sake of brevity, we illustrate with the simplest examples, though there are many to be found. Take, for example, any odd cycle C_{2k+1}. This graph clearly has a non-trivial automorphism, but $\Psi = (C_{2k+1}, \psi)$ is spectrally symmetric only when $\phi(\Psi) = \pm i$. Moreover, taking an arbitrary asymmetric graph G and assigning each of its edges a strictly imaginary gain yields a spectrally symmetric gain graph, disproving the reverse implication.

Next, it is easy to see that sign-symmetry of Ψ implies the structural symmetry of its underlying graph $\Gamma(\Psi)$, unless every odd cycle has strictly imaginary gain.

Proposition 6.3. *If the gain graph Ψ is sign-symmetric then either $\Gamma(\Psi)$ is symmetric or every odd cycle C in Ψ has $Re\left(\phi(C)\right) = 0$.*

Proof. Suppose that Ψ is switching isomorphic to $-\Psi$, i.e., $A(\Psi) = XP(-A(\Psi))P^{-1}X^{-1}$ for some diagonal matrix X with $X_{jj} \in \mathbb{T}$ for all j and some permutation matrix P. Moreover, suppose that at least one odd cycle C has $\mathrm{Re}\left(\phi(C)\right) \neq 0$. Then $\mathrm{Re}\left(\phi(C_\Psi)\right) \neq \mathrm{Re}\left(\phi(C_{-\Psi})\right)$, so P is not the identity. Then $\Gamma(\Psi)$ is not asymmetric since there exists an automorphism of $\Gamma(\Psi)$. Indeed, $\Gamma(\Psi) = P\Gamma(\Psi)P^{-1}$. □

The reverse implication does not hold. This is easy to see, by taking any symmetric non-bipartite graph G and choosing the all-one gain function $\mathbf{1}$. Then $\Psi = (G, \mathbf{1})$ contains at least one odd cycle with gain 1, but no odd cycles with gain -1. Thus, the conclusion follows by Lemma 6.2. For more detail regarding the case that $\mathrm{Re}\left(\phi(C)\right) = 0$, see Section 6.3.2.

Finally, sign-symmetry clearly implies spectral symmetry.

Lemma 6.4. *If $\Psi = (G, \psi)$ is sign-symmetric, then its spectrum is also symmetric.*

Proof. By construction λ occurs as an eigenvalue of $A(\Psi)$ if and only if $-\lambda$ occurs as an eigenvalue of $A(-\Psi) = -A(\Psi)$, and since switching equivalence of two gain graphs implies that their spectra coincide, it follows that $\Psi \sim -\Psi$ implies $\{\lambda_1, \lambda_2, \ldots, \lambda_n\} = \{-\lambda_n, -\lambda_{n-1}, \ldots, -\lambda_1\}$. □

The reverse is not necessarily true, though examples to attest to this fact have historically been difficult to find. Some signed graph examples can be found in [42], and the remainder of this work will be dedicated to finding a much larger family of gain graphs with this property, which is ultimately found and discussed in Theorem 6.17.

6.3 Spectral symmetry

In order to understand the possibility for spectral symmetry without sign-symmetry, it stands to reason that one must first have a firm grasp of the circumstances required for the former to occur. In particular, we investigate whether or not any graph allows a symmetric spectrum, and which graphs require it.

6.3.1 Necessary sign-symmetry

Probably the first result that one learns about in a spectral graph theory course is the well-known theorem that a graph has a symmetric spectrum if and only if it is bipartite. We find a largely similar result in the context of gain graphs. Indeed, without too much effort, one may show that all Ψ on G are spectrally symmetric if and only if G is bipartite.

Lemma 6.5. *If G is bipartite, then any Ψ with $\Gamma(\Psi) \cong G$ is sign-symmetric, and thus spectrally symmetric.*

Proof. Let $-\Psi = (G, \psi')$, where $\psi'(uv) = -\psi(uv)$. If G is bipartite then every cycle $C \in \mathcal{C}(G)$ satisfies $\phi'(C) = (-1)^{|C|}\phi(C) = \phi(C)$. By Theorem 4.3, we thus have $\Psi \sim -\Psi$, so Ψ is indeed sign-symmetric. □

Proposition 6.6. *The graph G requires symmetric gain-spectra if and only if G is bipartite*

Proof. Sufficiency follows from Lemma 6.5. In order to see necessity, assume to the contrary that G is not bipartite. Then G is, itself, a gain graph (with the all-ones signature). Since G is not bipartite, its adjacency spectrum is not symmetric, and the claim follows. □

The above may be reformulated in an interesting manner.

Corollary 6.6.1. *The graph G requires symmetric gain-spectra if and only if G itself has a symmetric spectrum.*

6.3.2 Allowed spectral symmetry

As was clear from Lemma 6.1 and Theorem 1.2, and even further illustrated by Proposition 6.6, a central role is played by odd cycles contained in our gain graphs. This section gradually considers some special cases of graphs that do contain odd cycles, to conclude that any graph allows a symmetric gain-spectrum.

In case only one odd cycle appears, it straightforwardly follows that the gain graph is spectrally symmetric if and only if said odd cycle has strictly imaginary gain.

Proposition 6.7. *Let Ψ be a non-bipartite gain graph and let $\Gamma(\Psi)$ be unicyclic. Then Ψ has a symmetric spectrum if and only if its cycle C satisfies $Re(\phi(C)) = 0$.*

Proof. Let C be the sole cycle in G, whose order m is odd. It should be clear that C constitutes the single order-m elementary subgraph of $\Gamma(\Psi)$. Hence

$$a_m = 2\mathrm{Re}\,(\phi(C)) = 0 \iff \mathrm{Re}\,(\phi(C)) = 0.$$

Furthermore, since any elementary subgraph of odd order $j > m$ must contain C, the contribution of said subgraph to a_j is multiplied with $\mathrm{Re}\,(\phi(C)) = 0$, hence, $a_j = 0$ follows. Finally, note that for any odd $j < m$, there exist no elementary spanning subgraphs of order j as there are no odd cycles of order at most j. $\square$

Moreover, note that the above still holds up when arbitrarily many even cycles occur.

Proposition 6.8. *Let Ψ be a gain graph with arbitrarily many even-sized cycles, but only a single odd-sized cycle C. Then Ψ has a symmetric spectrum if and only if $Re\,(\phi(C)) = 0$.*

An interesting distinction between the two propositions above should be mentioned here. Note that the graphs in Proposition 6.7 have the gains of their entire cycle space determined by the demand for spectral symmetry. That is, a unicyclic graph allows a spectrally symmetric gain graph, but any such gain graph belongs to the same switching equivalence class. By contrast, while the odd cycle of the gain graphs in Proposition 6.8 is 'locked' to $\pm i$, the remaining cycles are all even and their gains are therefore of no consequence to the symmetry of the spectrum. Since the gain of at least one such even cycle may be freely chosen, it then follows from Theorem 4.3 that infinitely many switching-distinct gain graphs with symmetric spectra occur on these underlying graphs. However, it should also be noted that graphs with exactly one odd cycle are reasonably rare. In particular, they either consist of exactly a single odd cycle or are not 2-connected; the latter is mainly relevant for Theorem 6.20. Section 6.5 will explore this situation in more detail.

The following can be shown analogously to Proposition 6.7.

Lemma 6.9. *Let Ψ be a gain graph whose odd-sized cycles C all satisfy $Re\,(\phi(C)) = 0$. Then the spectrum of Ψ is symmetric.*

Note that the reverse need not be true, as is the case in Figure 6.2. A straightforward application of Lemma 6.9 leads to the conclusion that any graph is underlying to at least one equivalence class of gain graphs whose spectra are symmetric.

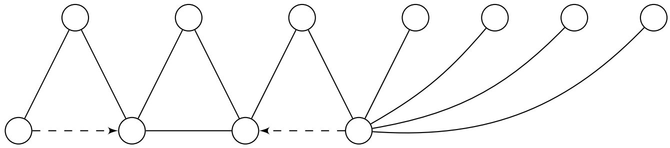


Figure 6.2 – A gain graph whose spectrum is symmetric. Here, the filled edges have gain 1 and the dashed arcs have gain $\exp(2i\pi/3)$. (Ocurred before as Figure 4.5)

Proposition 6.10. *Any graph G allows a symmetric gain-spectrum.*

Proof. Let G be a graph and let Ψ be the gain graph obtained from G by assigning strictly imaginary gain to any edge in $E(G)$. Then any odd cycle C in Ψ has $\mathrm{Re}\,(\phi(C)) = 0$, and the conclusion follows by Lemma 6.9. □

Note, however, that this brings us no closer to finding families of gain graphs whose spectral symmetry does not imply sign-symmetry. Indeed, any gain graph all of whose odd cycles have strictly imaginary gain is, again, necessarily sign-symmetric.

Lemma 6.11. *Let Ψ be a gain graph with $Re\,(\phi(C)) = 0$ for every odd cycle C. Then Ψ is sign-symmetric.*

Proof. Observe that the gain of every even cycle is unaffected by the negation, as in the bipartite case. Moreover, the odd cycles all have a zero real part, which is therefore also unchanged. □

The above should be somewhat expected to the experienced reader, as it was effectively previously observed by Guo and Mohar [51] in the context of Hermitian adjacency matrices. Nevertheless, it is a good example of the ways in which this much more general setting differs from circumstances in which the original question was posed.

6.4 Constructions

The logical question that follows from the above asks if we can construct spectrally symmetric graphs with at least one odd cycle whose gain has a nonzero real part. Clearly, the contribution of such an odd cycle must be counteracted by the contributions of other (possibly smaller) odd cycles, in such a way that their respective contributions to all odd a_j are, in a sense, balanced. The easiest way to accomplish this would be to simply take the disjoint union of Ψ and $-\Psi$. In order to find graphs which are connected, we must be a bit more resourceful.

The idea of effectively joining Ψ and $-\Psi$ together to obtain a single spectrally symmetric gain graph is quite similar to the ideas applied in various constructions of Hadamard matrices [100, 65], weighing matrices [8] and constructions of e.g. cubic graphs [2]. For example, the following is a straightforward generalization of a result by Ghorbani et al. [42].

Lemma 6.12 ([42]). *Let Ψ be an arbitrary gain graph, and denote $A = A(\Psi)$ and B be a Hermitian n-by-n matrix. Then $\tilde{\Psi}$, obtained from Ψ as*

$$A(\tilde{\Psi}) = \begin{bmatrix} A & B \\ B^* & -A \end{bmatrix}$$

has a symmetric spectrum. Moreover, $\tilde{\Psi}$ is sign-symmetric.

Proof. Let $P = \begin{bmatrix} O & I \\ I & O \end{bmatrix}$ and $X = \begin{bmatrix} -I & O \\ O & I \end{bmatrix}$. Then

$$PXA(\tilde{\Psi})X^{-1}P^{-1} = \begin{bmatrix} -A & -B \\ -B^* & A \end{bmatrix} = -A(\tilde{\Psi}),$$

and thus $A(\tilde{\Psi}) \sim -A(\tilde{\Psi})$. □

In case B is not Hermitian, the switching isomorphism above does not work in general, as is illustrated in the following example.

Example 6.1. *Let A be Hermitian $n \times n$, let B be non-Hermitian with $B = C + zI$ for some Hermitian C and $z \in \mathbb{T} \setminus \{\pm 1\}$, and X and P as above. Then*

$$\begin{aligned} -\begin{bmatrix} A & B \\ B^* & -A \end{bmatrix} &= \begin{bmatrix} -A & -C - zI \\ -C^* - \bar{z}I & A \end{bmatrix} \\ &\neq \begin{bmatrix} -A & -C - \bar{z}I \\ -C^* - zI & A \end{bmatrix} = PX \begin{bmatrix} A & B \\ B^* & -A \end{bmatrix} X^{-1}P^{-1}. \end{aligned}$$

As an aside, note that if A and C are strictly real, then the two matrices are still switching equivalent, as the switching classes are closed under transposition, by definition.

However, in case the off-diagonal blocks are not Hermitian, one may still apply similar block constructions. The attentive reader may notice a similarity to the doubling operation used by Huang [65] to construct signed n-cubes. This construction may indeed be used to obtain gain graphs with symmetric spectra.

Lemma 6.13. *Let Ψ be an arbitrary order-n gain graph, denote $A = A(\Psi)$ and let $z \in \mathbb{T}$. Then $\hat{\Psi}$, defined by $A(\hat{\Psi}) = \begin{bmatrix} A & zI \\ \bar{z}I & -A \end{bmatrix}$, is sign-symmetric.*

Proof. In the following, recall that addition of vertex indices is modulo $2n$. Then, by construction, for every odd cycle C, whose (ordered) vertices are $v_{u_1}, v_{u_2}, \ldots, v_{u_k}$, the cycle C' with vertices $v_{u_1+n}, v_{u_2+n}, \ldots, v_{u_k+n}$, is such that $\phi(C) = -\phi(C')$. Hence, Ψ is isomorphic to $-\Psi$. □

The above are all even-order gain graphs. Of course, one may obtain the same kind of symmetry with a central $(2n+1)$th vertex. To illustrate, we include the following construction.

Lemma 6.14. *Let Ψ be an arbitrary gain graph, and denote $A(\Psi) = \begin{bmatrix} 0 & a \\ a^* & A' \end{bmatrix}$. Then $\hat{\Psi}$, obtained from Ψ as $A(\hat{\Psi}) = \begin{bmatrix} 0 & a & -a \\ a^* & A' & O \\ -a^* & O & -A' \end{bmatrix}$ is sign-symmetric.*

The above yields plenty of spectrally symmetric gain graphs. The main drawback of the constructions above, for the purposes of this article, is that they are also all sign-symmetric. However, inspired by Example 6.1, we arrive at another construction, the foundation of which is known as Sylvester's double. Effectively, we more or less use a hybrid of Lemmas 6.12 and 6.13 to turn an arbitrary gain graph into a spectrally symmetric one.

Lemma 6.15. *Let Ψ be an arbitrary gain graph, denote $A = A(\Psi)$ and let $z \in \mathbb{T} \cup \{0\}$. Then $\breve{\Psi}$, defined by*

$$A(\breve{\Psi}) = \begin{bmatrix} A & A + zI \\ A + \bar{z}I & -A \end{bmatrix}, \tag{6.1}$$

has a symmetric spectrum.

Proof. Let $M = \begin{bmatrix} A & A+zI \\ A+\bar{z}I & -A \end{bmatrix}$. Then, we have

$$\begin{aligned}\det(M-\mu I) &= \det\left(\begin{bmatrix} A-\mu I & A+zI \\ A+\bar{z}I & -A-\mu I \end{bmatrix}\right) \\ &= \det((A-\mu I)(-A-\mu I) - (A+zI)(A+\bar{z}I)) \\ &= \det(-A^2+\mu^2 I - (A+zI)(A+\bar{z}I)),\end{aligned}$$

where the second equality holds since $A+\bar{z}I$ and $A-\mu I$ commute. Since μ appears in the final expression only as μ^2, no odd-powered terms appear in the characteristic polynomial and thus the spectrum is symmetric. □

The key difference of Lemma 6.15 compared to the constructions that appeared before, is that one does not necessarily have sign-symmetry. An example is provided below.

Example 6.2. *Let $c \in \mathbb{T}$ and $\omega = \exp(i\pi/3)$. Define*

$$A = \begin{bmatrix} 0 & 1 & 1 & \bar{\omega} & \bar{\omega}^2 \\ 1 & 0 & \bar{\omega}^2 & \bar{\omega}^2 & 0 \\ 1 & \omega^2 & 0 & 0 & \bar{\omega}^2 \\ \omega & \omega^2 & 0 & 0 & 0 \\ \omega^2 & 0 & \omega^2 & 0 & 0 \end{bmatrix} \text{ and } M = \begin{bmatrix} A & A+zI \\ A+\bar{z}I & -A. \end{bmatrix}$$

Let $z = \exp(i\pi/5)$. Then M contains 628 nine-cycles with real part $-\frac{1}{2}(\sqrt{3}\ Im(z) + Re(z))$ and only 620 with real part $\frac{1}{2}(\sqrt{3}\ Im(z) + Re(z))$. It follows by Lemma 6.2 that M is not sign-symmetric. The same conclusion holds for any $z \in \mathbb{T}$, though the exact count may differ. This fairly tedious matter of counting has been verified by computer.

In fact, we may abuse the fact that the off-diagonal blocks are not Hermitian to conclude that the above construction is, in general, not sign-symmetric.

Theorem 6.16. *Let Ψ be a connected nonbipartite gain graph with $\Gamma(\Psi)$ asymmetric, denote $A = A(\Psi)$ and let $z \in \mathbb{T} \setminus \mathbb{T}_4$. Then $\breve{\Psi}$, defined by $M := A(\breve{\Psi}) = \begin{bmatrix} A & A+zI \\ A+\bar{z}I & -A \end{bmatrix}$, is sign-symmetric if and only if Ψ is switching equivalent to a signed graph.*

Proof. Suppose that Ψ is switching equivalent to a signed graph. Then, w.l.o.g., it may switched such that the entries of $A(\Psi)$ are all real. Let $P = \begin{bmatrix} O & I \\ I & O \end{bmatrix}$ and $X = \begin{bmatrix} -I & O \\ O & I \end{bmatrix}$. Then

$$PXMX^{-1}P^{-1} = \begin{bmatrix} -A & -A - \bar{z}I \\ -A - zI & A \end{bmatrix} = -M^\top. \tag{6.2}$$

Since switching isomorphism classes are by definition closed under taking the converse, this shows that $M \sim -M$. Note that taking the transpose only affects the diagonal entries of the off-diagonal blocks, since A is strictly real and thus symmetric.

We consider the reverse implication. By construction,

$$\Gamma(M) = \begin{bmatrix} |A| & |A| + I \\ |A| + I & |A| \end{bmatrix}$$

has precisely the full automorphism group generated by all of the transpositions $(v, v+n)$, with $v \in [n]$, where n is the order or Ψ. Since a switching isomorphism from M to $-M$ is an automorphism of $\Gamma(M)$, it therefore follows that the permutation matrix P, representing the relabeling of the vertices, is symmetric. That is, $P^2 = I$.

Note that since Ψ is nonbipartite, there is at least an odd cycle C' in $\breve{\Psi}$ whose gain is affected by the negation, i.e., $\operatorname{Re}(\phi(C')) \neq 0$. Indeed, if all odd cycles in Ψ would be strictly imaginary; one could take an odd cycle $C = (v_{c_1}, v_{c_2}, \ldots, v_{c_k})$ from Ψ and add two vertices from the negated copy to obtain $C' = (v_{c_1}, v_{c_1+n}, v_{c_2}, v_{c_2+n}, v_{c_3}, v_{c_4}, \ldots, v_{c_k})$. Then $\phi(C') = z^2\phi(C)$, and thus $\operatorname{Re}(\phi(C')) \neq 0$, showing our claim. Since switching does not affect the gain of a cycle, $M \sim -M$ now implies $P \neq I$.

Assume, for now, that we do not take the converse. Then there are some matrices P, X such that $PXMX^{-1}P^{-1} = -M$, where P is a (non-identity) symmetric permutation matrix and X is a diagonal matrix whose diagonal entries are complex units. Let $\mathcal{R} \subseteq V$ denote the vertices that are not fixed by P. Observe that $|\mathcal{R}| = 0$ implies $P = I$, which contradicts the above. Assume without loss of generality that $\mathcal{R} = \{1, \ldots, r\}$ for some $1 \leq r < n$ (the case $r = n$ is treated later), and decompose A as

$$A = \begin{bmatrix} A_R & B \\ B^* & A_F \end{bmatrix},$$

where $A_R \in \mathbb{C}^{r \times r}$ and the remaining blocks are appropriately dimensioned. Accordingly decompose X as $X = diag(X_R, X_F, Y_R, Y_F)$, where $X_R, Y_R \in \mathbb{C}^{r \times r}$ and $X_F, Y_F \in \mathbb{C}^{n-r \times n-r}$. Then

$$M' := PXA(\breve{\Psi})X^{-1}P^{-1} = \tag{6.3}$$
$$\begin{bmatrix} -Y_R A_R Y_R^{-1} & Y_R B X_F^{-1} & Y_R(A_R + \bar{z}I)X_R^{-1} & -Y_R B Y_F^{-1} \\ X_F B^* Y_R^{-1} & X_F A_F X_F^{-1} & X_F B^* X_R^{-1} & X_F(A_F + zI)Y_F^{-1} \\ X_R(A_R + zI)Y_R^{-1} & X_R B X_F^{-1} & X_R A_R X_R^{-1} & X_R B Y_F^{-1} \\ -Y_F B^* Y_R^{-1} & Y_F(A_F + \bar{z}I)X_F^{-1} & Y_F B^* X_R^{-1} & -Y_F A_F Y_F^{-1} \end{bmatrix},$$

which equals $-M$ on all entries. Observe from the (1,3) block that $\bar{z}Y_R X_R^{-1} = -zI$, and thus $Y_R = -z^2 X_R$. Furthermore, from blocks (1,2) and (3,2), we have $Y_R B X_F^{-1} = -B = X_R B X_F^{-1}$. Now, since B is non-zero (otherwise Ψ is not connected), these two equations jointly imply $z^2 = -1$, which is a contradiction.

What remains is to consider $r = n$. Then similarly to before

$$M' = \begin{bmatrix} -X_R A_R X_R^{-1} & -z^2 X_R(A_R + \bar{z}I)X_R^{-1} \\ -\bar{z}^2 X_R(A_R + zI)X_R^{-1} & X_R A_R X_R^{-1} \end{bmatrix}, \tag{6.4}$$

and thus $-X_R A_R X_R^{-1} = -A_R$ and $-z^2 X_R A_R X_R^{-1} = -A_R$, which in this case implies $z^2 = 1$ since A_R is non-zero. This is again a contradiction.

Finally, we revisit the matter of taking the converse. Let $1 \leq r < n$ and, contrary to before, suppose now that $M' = -M^\top$, where M' is as in (6.3). Then $\bar{z}Y_R X_R^{-1} = -\bar{z}I$ and thus $X_R = -Y_R$. Note the similarity to before; a parallel argument may be formulated with little effort.

In case $r = n$, some extra effort is needed. Plugging in $X_R = -Y_R$ into (6.3) and equating the result to $-M^\top$ yields $X_R A_R X_R^{-1} = A_R^\top$, which is equivalent to

$$[X_R]_{uu} A_{uv} [X_R]_{vv}^{-1} = \overline{A_{uv}} \quad \forall (u, v) \in E. \tag{6.5}$$

Note that if $A_{uv} = 1$, then it clearly follows that $[X_R]_{uu} = [X_R]_{vv}$. Now, since one may without loss of generality assume (see Corollary 4.4.1) that a spanning tree of the edges has gain 1, it follows that $X_R = cI$ for some $c \in \mathbb{T}$. But then (6.5) reduces to $A_{uv} = \overline{A_{uv}}$, which implies $A \in \mathbb{R}^{n \times n}$ and is therefore switching equivalent to a signed graph. $\square$

Using Lemma 6.15 and Theorem 6.16, we thus obtain a huge family of gain graphs that are spectrally symmetric but not sign-symmetric. In particular, since there is substantial freedom in the choice of Ψ, there should be examples of such gain graphs with many graph theoretical properties. In light of the comparatively narrow families of signed graphs presented by Ghorbani et al. [42], this is quite surprising. The following should be clear.

Theorem 6.17. *For almost every gain graph Ψ and $c \in \mathbb{T}$, its double $\breve{\Psi}$ as constructed in* (6.1) *is spectrally symmetric and structurally symmetric, but not sign-symmetric.*

6.5 An open problem concerning the general case

While Theorem 6.17 yields an abundance of examples, we have reason to believe that spectral symmetry without sign-symmetry occurs much more widely. With extensive numerical exploration, including but not limited to the trials discussed in Section 5.4.2, we find that most sufficiently dense graphs allow many switching-distinct gain graphs with symmetric spectra. It has proved difficult to formulate a convincing argument for the general case, but we choose to include our expectations in the hopes of attracting attention to this interesting question.

At the heart of the following discussion is the cycle space $\mathcal{C}$ of a graph and its dimension[1] $\dim \mathcal{C} = |\mathcal{B}|$, relative to the order of the graph. We recall the following fact.

Lemma 6.18. *Let $\Psi = (G, \psi)$ be a connected gain graph. Then $\dim \mathcal{C}(\Psi)$ is equal to $m - n + 1$.*

Proof. Let T be a spanning tree of G. Then there are $m - n + 1$ (not necessarily disjoint) cycles consisting of exactly one edge outside of T and a number of of edges inside T; these are called *fundamental* cycles. Since every cycle in G may be obtained as the symmetric difference of fundamental cycles, these cycles form a basis. $\square$

6.5.1 Even cycles in a cycle basis

Initially, one is inclined to use the observation that the gain of an even cycle is much less restricted by the desire for spectral symmetry. However, one quickly encounters a problem that was eluded to following Proposition 6.8.

[1] Recall that $\mathcal{B}$ denotes the basis of the cycle space.

Lemma 6.19. *Let G be such that every basis of its cycle space contains an even-order cycle. Then there are infinitely many switching equivalence classes on G, whose spectra are symmetric.*

Proof. let $\mathcal{C}$ be an arbitrary basis of the cycle space of G, and construct Ψ by choosing the gains of all odd cycles in $\mathcal{C}$ to be strictly imaginary. Then, independently of the gains of the even cycles in $\mathcal{C}$, the spectrum of Ψ is symmetric. Since two gain graphs are switching equivalent if and only if (the real parts of) their gains coincide on a basis of the cycle space, the remaining freedom of choice for the gains of the even cycles yields infinitely many switching equivalence classes, as desired. □

Interestingly, the requirement in Lemma 6.19 is very rarely met: it would require the graph to not be 2-connected. That is, the graph be such that removal of a single vertex would yield a disconnected graph. Clearly, such a vertex is unlikely to occur in a large random graph, thus invalidating Lemma 6.19 as a piece of machinery fit for analysis of the asymptotic case.

Theorem 6.20 (Henning and Little [63])**.** *Every 2-connected nonbipartite graph has a cycle basis consisting only of odd cycles.*

Proof. (*Sketch.*) Start with an odd cycle C_1, and pick a cycle C_2 that coincides with C_1 on at least an edge. Now either C_2 is odd or C_2 is even. In the latter case, C_2', obtained as the symmetric difference of C_1 and C_2, is odd. One may continue in this way to obtain an odd cycle basis, provided that the graph is 2-connected. □

6.5.2 A system of polynomial equations

Once more, the central issue seems to be the age-old question of a number of solutions to a given system of equations. Indeed, note that since the gain of every cycle in a gain graph may be written as a product of the gains of cycles from a (fundamental) cycle basis, constructing a gain function that equips a given underlying graph with a symmetric gain-spectrum essentially corresponds to solving the system of equations $a_{2k+1} = 0$, $2k+1 \leq n$, $k \in \mathbb{N}$. If the cycle space is relatively small, this may lead to a system with finitely many solutions.

Example 6.3. *Consider the graph in Figure 6.3a. Its cycle space consists of two independent triangles whose gains are α and β. By applying Theorem 1.2, it follows*

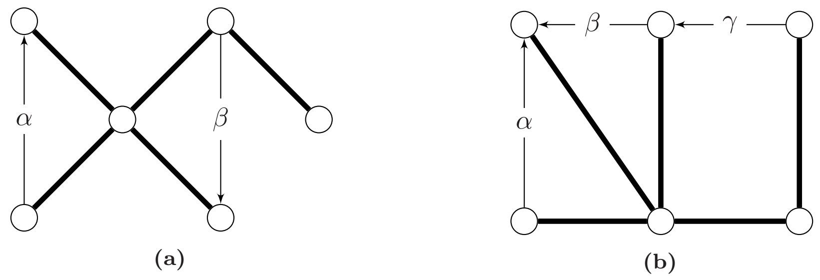


Figure 6.3 – Illustrations for Examples 6.3 and 6.4. Fat edges may w.l.o.g. be assumed to have gain 1. Only the 'forward' arc of every remaining pair is illustrated.

that the corresponding gain graph is spectrally symmetric if and only if

$$\begin{cases} -2Re\,(\alpha) - 2Re\,(\beta) = 0 \\ 4Re\,(\alpha) + 2Re\,(\beta) = 0, \end{cases}$$

which implies $\alpha = \pm i$ and $\beta = \pm i$. These options leave at most four distinct gain graphs; in this particular case, they are all equivalent.

Note that if the rightmost vertex were removed, then the corresponding gain graph would be spectrally symmetric for any $\alpha = -\beta$. Indeed, in this case, the two triangles would be symmetric to one-another, which translates to dependency in the system of equations above.

Formalizing the idea in the example above leads to the following intuitive result.

Proposition 6.21. *Let G be connected and asymmetric with $m \leq \frac{3}{2}(n-1)$. Then G allows finitely many switching-distinct gain graphs with symmetric spectra.*

Proof. Let $\mathcal{B}$ be a cycle basis of G of size $b = m - n + 1 =$. For every $C_j \in \mathcal{B}$, apply a common change of variable by setting $\phi(C_j) = r_j + iq_j$, with $r_j, q_j \in \mathbb{R}$. Clearly, since $|\phi(C_j)| = 1$, it should also hold that $r_j^2 + q_j^2 = 1$ for all $j = 1, \ldots, b$.

Consider an order-k elementary subgraph H of G. By Theorem 1.2, the contribution of H to a_k is dependent on the gains of the cycles in H; specifically, on

$\prod_{C\in\mathcal{C}(H)} \mathrm{Re}\,(\phi(C))$. Since $\phi(C)$ may be expressed as[2]

$$\phi(C) = \prod_{C_j\in\mathcal{B}^{\rightarrow}(C)} \phi(C_j) \prod_{C_j\in\mathcal{B}^{\leftarrow}(C)} \overline{\phi(C_j)} = \prod_{C_j\in\mathcal{B}^{\rightarrow}(C)} (r_j + iq_j) \prod_{C_j\in\mathcal{B}^{\leftarrow}(C)} (r_j - iq_j), \tag{6.6}$$

it should be clear that

$$\mathrm{Re}\,(\phi(C)) = f_C(r_1,\ldots,r_b,q_1,\ldots,q_b)$$

for some real polynomial f_C.Because this applies for every cycle C in every elementary subgraph H of every order k, it follows that every coefficient a_k is a polynomial in $r_1,\ldots,r_B,q_1,\ldots,q_B$. By collecting all of the above, we obtain the following system of simultaneous equations:

$$\begin{cases} a_k(r_1,\ldots,r_B,q_1,\ldots,q_B) = 0 & \text{for all } 3\le k\le n, k \text{ odd} \\ r_j^2 + q_j^2 = 1 & \text{for all } j = 1,\ldots,B. \end{cases} \tag{6.7}$$

Note that this system contains $(n-1)/2 + B$ equalities and $2B$ real-valued variables. Additionally, since G is asymmetric, it follows that the equations are linearly independent. Now, since $2B - ((n-1)/2 + B) = m - \frac{3}{2}(n-1) \le 0$ by assumption, this system of polynomial equations has at most as many variables as equalities. Hence, the system has finitely many solutions over the complexes [82, Thm. 14.1]; implicitly, it also has finitely many solutions over the reals. □

Conversely, if the cycle space is of sufficiently high dimension, this leads to a system of equations that has more variables than equations, which is often associated with infinitely many solutions.

Example 6.4. *Consider the graph in Figure 6.3b. Again, its spectrum is symmetric if and only if the following system of simultaneous equations holds:*

$$\begin{cases} -2Re\,(\alpha) - 2Re\,(\beta) = 0 \\ 4Re\,(\alpha) + 2Re\,(\beta) - 2Re\,(\beta\gamma) = 0 \end{cases}$$

[2] Here, $\mathcal{B}^{\rightarrow}(C), \mathcal{B}^{\leftarrow}(C) \subseteq \mathcal{B}$ are the basis cycles traversed respectively "clockwise" and "anticlockwise" to obtain C. Recall that in order for the gain of a constructed cycle to be the product of the gains of the constructing cycles, their intersection must be traversed in opposing directions.

with $\alpha, \beta, \gamma \in \mathbb{T}$. As in the proof of Proposition 6.21, this can be turned into

$$\begin{cases} -2r_1 - 2r_2 = 0 \\ 4r_1 + 2r_2 - 2(r_2 r_3 - q_2 q_3) = 0 \\ r_1^2 + q_1^2 = 1 \\ r_2^2 + q_2^2 = 1 \\ r_3^2 + q_3^2 = 1. \end{cases}$$

Since this system of polynomial equations has strictly more variables than equalities, it has infinitely many solutions over an algebraically closed field. Regrettably, the later system has real-values variables by the applied change of variables, so this argument does not apply.

Nevertheless, one can still conclude that any solution with $r_1 \in [-1, 1], r_2 = -r_1, r_3 = -1$, with appropriate q_1, q_2, q_3, solves the system. Since the gains of the fundamental cycle basis may take infinitely many distinct values, it follows by Theorem 4.3 that there are infinitely many switching distinct gain graphs with symmetric spectra on this underlying graph.

This then leads to the following question.

Question 6.1. *Is it true that a graph G allows finitely many switching-distinct gain graphs with symmetric spectra only if $|E(G)| \leq m^*$, for some $m^* \in \mathbb{N}$? In particular, does the bound $m^* = \frac{3}{2}(n-1)$ apply?*

Numerical testing has thus far not given us a reason to believe that the statement should be more nuanced than above, though that is, of course, a possibility. While one may formalize by hand on a case-by-case basis, as in Example 6.4, a conclusive answer to the general question unfortunately still eludes us.

6.5.3 Asymptotic consequence

The above has some interesting repercussions for the existence of gain graphs whose spectral symmetry does not imply sign-symmetry. In particular, recall from Proposition 6.3 that a (non-bipartite) sign-symmetric gain graph is necessarily structurally symmetric. One could then be easily convinced of the following conclusion.

Proposition 6.22. *If Question 6.1 can be positively answered on both counts, then almost all graphs allows infinitely many switching-distinct gain graphs whose spectra* *are symmetric, but which are not sign-symmetric.*

Proof. It is well-known that almost every graph is asymmetric; see Chapter 3. Thus, we may consider the probability that a random Erdős-Rényi graph $G(n, p = 1/2)$ satisfies the bound mentioned in Question 6.1, to arrive at the desired conclusion. Let X_j be independent Bernoulli variables with $\mathbb{P}(X_j = 1) = \frac{1}{2}$ and let

$$X = \sum_{j=1}^{n(n-1)/2} X_j. \tag{6.8}$$

Then, with $\delta = 1 - \frac{6}{n}$ and $\mu = \mathbb{E}(X) = n(n-1)/4$, we have:

$$\begin{aligned}
\mathbb{P}\left(X \leq \frac{3(n-1)}{2}\right) &= \mathbb{P}(X \leq (1-\delta)\mu) && (6.9)\\
&\leq \exp\left(-\frac{1}{2}\delta^2\mu\right) && (6.10)\\
&= \exp\left(-\frac{1}{4}\left(n^2 - 13n + 48 - 36n^{-1}\right)\right), && (6.11)
\end{aligned}$$

which clearly tends to 0 as n goes to infinity. Here, (6.10) follows by application of the Chernoff bound (see Theorem 3.1). □

To conclude, we note that the conclusion of Proposition 6.22 would be, in some respect, quite surprising. Indeed, the matter of signed graphs that are not sign-symmetric, but whose spectra are symmetric, turned out to be quite formidable question that was listed as an open problem in [6] and answered by [42]. While one has much more freedom to work with in the gain graph paradigm, it does seem remarkable that gain graphs that satisfy the above property appear so bountifully.

CHAPTER 7

Unit gain graphs with two distinct eigenvalues

Abstract

Since the introduction of the Hermitian adjacency matrix for digraphs, interest in so-called complex unit gain graphs has surged. In this chapter, we consider gain graphs whose spectra contain the minimum number of two distinct eigenvalues. Analogously to graphs with few distinct eigenvalues, a great deal of structural symmetry is required for a gain graph to attain this minimum. This allows us to draw a surprising parallel to well-studied systems of lines in complex space, through a natural correspondence to unit-norm tight frames. We offer a full classification of two-eigenvalue gain graphs with degree at most 4, or with multiplicity at most 3. Intermediate results include an extensive review of various relevant concepts related to lines in complex space, including SIC-POVMs, MUBs and geometries such as the Coxeter-Todd lattice, and many examples obtained as induced subgraphs by employing a technique parallel to the dismantling of association schemes. Finally, we touch on an innovative application of Simulated Annealing to find examples by computer.

7.1 Introduction

An especially captivating line of research considers graphs, whose associated matrices have few distinct eigenvalues. Such graphs are generally highly structurally symmetric, which allows for a beautiful interplay of algebra and combinatorics. A non-empty graph must always have at least two distinct eigenvalues; a bound that is essentially only attained in a complete graph. In this chapter, we explore the degree to which this holds true for modern alternatives to the classical binary graphs, and investigate the necessary circumstances for such generalizations to yield examples outside of their immediate graph parallels.

Recently, Belardo et al. [6] posed the problem of investigating signed graphs with exactly two distinct eigenvalues. Quite a few papers have since appeared on the topic. In particular, Huang [65] has used a construction of signed n-cubes with exactly two eigenvalues in his recent proof of the so-called Sensitivity Conjecture of Nisan and Szegedy on Boolean functions. Furthermore, Ramezani [90] applies the star-complement technique to find infinitely many k-regular signed graphs with two distinct eigenvalues $\pm\sqrt{k}$, with $k = 5, 6, \ldots, 10$, and Stanić [101] offers various theoretical and computational results, among others completing the list of 3- and 4-regular signed graphs with two distinct eigenvalues. Lastly, in an earlier work classifying cyclotomic matrices, Greaves [45] has obtained several infinite such families with two eigenvalues, slightly restricted versions of which can be interpreted as unit gain graphs.

In this work, we will further develop the ideas and results on signed graphs, above, to the more general setting of complex unit gain graphs. Many (or in fact all) such graphs that have exactly two eigenvalues correspond to interesting systems of lines in complex space, such that the angle between every non-orthogonal pair of lines is equal to some given constant. If every such line is represented by a vector with a given norm (say, 1), then one obtains an object known as an equal-norm tight frame [106]. Moreover, if no two such vectors are orthogonal, the system is said to be equiangular.

Due to their rich theoretical properties and their numerous practical applications, equiangular tight frames are arguably the most important class of finite-dimensional tight frames, and they are the natural choice when one tries to combine the advantages of orthonormal bases with the concept of redundancy provided by frames [102]. While most research regarding equiangular lines is relatively old (frames were used to analyze wavelets in the 1980s, e.g., [80]), the quantum computing community has been increasingly interested in equiangular tight frames, especially in the context of *sym-*

metric, informationally complete, positive operator-valued measures (SIC-POVM), which is a prominent candidate for a "standard quantum measurement," (see, e.g., [53, 54].) It has been shown to have applications in quantum state tomography [17] and quantum cryptography [40]. Furthermore, such SIC-POVM's are equivalent to equiangular tight frames of d^2 vectors in $\mathbb{C}^d$, and their existence for arbitrary d is one of the important open problems of the moment in quantum computing.

Our ultimate goal is to classify various families of unit gain graphs, with two distinct eigenvalues. The applied approach is twofold. Specifically, the combinatorially oriented graph perspective is focused on the degree of said graphs, while the lines perspective, that focuses on the multiplicities of eigenvalues, is more algebraically oriented. For gain graphs of degree at most four, we are able to completely characterize the collection of desired unit gain graphs. Some of these collections have infinitely many switching-distinct members, for given order and degree. The lines perspective also produces an abundance of interesting examples, and a complete characterization with least multiplicity at most 3 is obtained. Moreover, various other examples stemming from well-known combinatorial objects such as the Coxeter-Todd lattice are discussed, as well as a technique that is parallel to the dismantling of association schemes, which is used to find many two-eigenvalue subgraphs.

This chapter is organized as follows. In Section 7.2, we provide a thorough introduction of the concepts used throughout. Section 7.3 is concerned with the recursive constructions that may be applied to grow arbitrarily large gain graphs with exactly two distinct eigenvalues. Next, Section 7.4 draws from the literature on systems of lines in complex space to construct various examples; Section 7.5 uses these insights to classify all two-eigenvalues gain graphs with small multiplicity. Section 7.6 provides classifications of unit gain graphs with restricted degree, taking the combinatorial perspective. Finally, in Section 5.2, we touch on an application of simulated annealing to search for the desired gain graphs by computer.

7.2 Preliminaries

For details regarding terminology and notation, the reader is referred to Section 1.1. We note explicitly that any of the (gain) graphs throughout this chapter are assumed to be connected, as all possibly disjoint two-eigenvalue gain graphs may be constructed by taking the disjoint union of two smaller such gain graphs whose distinct eigenvalues coincide.

7.2.1 Two distinct eigenvalues

The main body of this work is concerned with gain graphs whose gain matrix has precisely two distinct eigenvalues; we will commonly call such objects *two-eigenvalue gain graphs*. Suppose that the two-eigenvalue gain graph Ψ has eigenvalues θ_1 and θ_2 with multiplicities m and $n-m$, respectively. If $a = \theta_1 + \theta_2$ and $k = -\theta_1\theta_2$, then the gain matrix A of Ψ satisfies

$$A^2 = aA + kI. \tag{7.1}$$

This implies that Ψ is k-regular, and hence that k is integer. Moreover, since clearly $k > 0$ (otherwise Ψ is the empty graph), A has full rank. Additionally, since A and $-A$ have opposite eigenvalues, we will consider without loss of generality only the case with $a \geq 0$, which since $\operatorname{Tr}(A) = 0$ implies $m \leq n/2$. Also note that $a \leq n-2$ with equality if and only if Ψ is switching equivalent to a complete graph, with distinct eigenvalues k and -1.

It is not hard to see that the eigenvalues of Ψ are the square roots of rational numbers. Indeed, using that $0 = \operatorname{Tr}(A) = m\theta_1 + (n-m)\theta_2$ and $nk = \operatorname{Tr}(A)^2 = m\theta_1^2 + (n-m)\theta_2^2$, it follows that

$$\theta_1 = \sqrt{\frac{k(n-m)}{m}} \quad \text{and} \quad \theta_2 = -\sqrt{\frac{km}{n-m}}.$$

Moreover, by applying the quadratic formula to (7.1), we also have

$$\theta_1 = \frac{a + \sqrt{a^2+4k}}{2} \quad \text{and} \quad \theta_2 = \frac{a - \sqrt{a^2+4k}}{2}.$$

If a is integer, the following result from Ramezani [89] carries over.

Lemma 7.1. *Let Ψ be a two-eigenvalue gain graph, and let $a \in \mathbb{Z}$. Then either*

(i) $a = 0$ and the eigenvalues are $\pm\sqrt{k}$, or

(ii) $a \neq 0$ and $a^2 + 4k$ is a perfect square,

Proof. The first part follows by plugging in $a = 0$ into (7.1). The second part is shown by contradiction. Suppose that $a^2 + 4k$ is not a perfect square, so that θ_1 is irrational. Then, since the characteristic polynomial of Ψ is a monic integral polynomial, the algebraic conjugate of θ_1, i.e., θ_2, occurs as an eigenvalue of A with the same multiplicity; say m. Now, since the trace of A equals zero, it follows that $m\theta_1 + m\theta_2 = ma = 0$, and hence $a = 0$, contradiction. □

Equivalently, one may formulate this in terms of n, m and k.

Lemma 7.2. *Let Ψ be a two-eigenvalue gain graph. If $a \in \mathbb{N}$ then $\frac{kn^2}{m(n-m)}$ is a perfect square.*

Proof. If $a > 0$, then by Lemma 7.1, $a^2 + 4k = b^2$, for some $b \in \mathbb{N}$. We may rewrite to obtain:

$$b^2 = a^2 + 4k = \left(\sqrt{k(n-m)m^{-1}} - k\left(\sqrt{k(n-m)m^{-1}}\right)^{-1}\right)^2 + 4k = \frac{kn^2}{m(n-m)}.$$

□

However, contrary to [89], the current context does not guarantee that a is integer. Consider the following example, constructed from an equiangular tight frame of 7 vectors in dimension 3, which is closely related to the Fano plane.

Example 7.1. *Let $A = \frac{1}{4}\sqrt{2}(I - J - i\sqrt{7}(N - N^\top))$, where*

$$N = CM\left(\begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 0 & 0 \end{bmatrix}\right).$$

Then $a = \frac{1}{2}\sqrt{2}$ and the eigenvalues of A are $2\sqrt{2}$ and $-\frac{3}{2}\sqrt{2}$. Moreover, note that $a^2 + 4k = 24\frac{1}{2}$, which is not a perfect square.

The construction in Example 7.1 is a member of an infinite family of gain graphs with two eigenvalues, that is based on a particular tight frame. Details regarding said family can be found in Section 7.4.4.

We end this preliminary section with an interesting tangent, concerning a line of research considers the spectral characterizations of (gain) graphs. A gain graph is said to be *determined by its spectrum* if it is switching isomorphic to any gain graph to which it is cospectral; a property that has not been much-researched in the context of gain graphs. It should then be noted that the two-eigenvalue gain graphs described in this work, have spectra that are extremely rare. By this observation, it stands to reason that a sizable number the two-eigenvalue gain graphs are, in fact, determined by their spectra. We will see in Sections 7.5 and 7.6 that this instinct is true. In an effort to keep the discussion focussed, we will not point out every instance of spectral determination, except in the summarizing Theorems 7.16 and 7.24.

(a) **(b)**

Figure 7.1 – Cospectral connected signed graphs, of which only (a) is regular.

7.2.2 Regularity in gain graphs

Unlike for its graph analog, regularity of a gain graph Ψ is not characterized by its spectrum. To see this, Belardo et al. [6] offer an example pair that are cospectral to one-another, while one is regular and the other is not. However, this pair does not feature two *connected* signed graphs.

It seems interesting to ask whether such examples may also be constructed under the assumption of connectedness. With relative ease, one finds a number of small examples to confirm the claim, even when both halves of the cospectral pair are required to be connected. Figure 7.1 illustrates one such example, though arbitrarily large ones may also be constructed. One such construction is provided below. Let $K_{p,q}$ be the complete bipartite graph, whose nonzero eigenvalues are $\pm\sqrt{pq}$ with multiplicity 1. Furthermore, let $K^*_{p,q,r}$ be a complete tripartite graph whose 3-cycles all have gain i and whose closed 4-walks all have gain 1; this graph has exactly two nonzero eigenvalues which are exactly $\pm\sqrt{pq+qr+rp}$.

Proposition 7.3 (Xu et al. [108])**.** *Let Γ be a connected graph and let $\Psi = (\Gamma, \psi)$ be a gain graph. Then Rank$(\Psi) = 2$ if and only if either $\Psi \sim K_{p,q}$ or $\Psi \sim K^*_{p,q,r}$.*

By using their respective spectra, as above, one finds the following.

Corollary 7.3.1. *Let m, j, s, t be natural numbers such that $m = j(s^2 + st + t^2)$. Then $K_{m,m}$ is cospectral to $K^*_{js^2,jt^2,j(s+t)^2}$.*

The above shows a construction of arbitrarily large pairs of connected gain graphs, of which exactly one (i.e., $K_{m,m}$) is regular, while the other not necessarily is. Note that this construction generalizes a remark that first appeared in [83].

As an aside, we note that one may characterize all gain graphs with rank 3 with a straightforward, though tedious, forbidden subgraph approach. This collection may loosely be described as all gain graphs switching equivalent to a twin expansion (see

Definition 2.7) of a triangle (not $K^*_{1,1,1}$) or a rank-3 gain graph on K_4. This has been proven by the author; the details are omitted.

7.3 Constructions

Somewhat unsurprisingly, there are various fairly well understood areas that are linked to the here considered notion. In this section, we will showcase these links and build on existing theory to obtain various two-eigenvalue gain graphs.

7.3.1 Weighing matrices

A complex unit weighing matrix is an $n \times n$ matrix W with entries in $\mathbb{T}$ such that $WW^* = kI$, for some k. Real weighing matrices have been quite extensively studied (see [58]), and their complex generalizations have recently been getting more and more attention, too. For example, Best et al. [8] characterized all complex unit weighing matrices (simply *weighing matrix,* hereafter) with weight at most 4.

Note that since a weighing matrix is square and $WW^* = W^*W = kI$, a Hermitian weighing matrix W with a zero diagonal characterizes a unit gain graph with eigenvalues $\pm\sqrt{k}$. The smallest nontrivial example of this is

$$W_4 = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & i & -i \\ 1 & -i & 0 & i \\ 1 & i & -i & 0 \end{bmatrix}.$$

Following a convention for Hadamard matrices [1], weighing matrices are said to be *graphical* when they are Hermitian and their diagonal is constant. This may only occur when the constant diagonal has value $\delta \in \{0, 1, -1\}$; the corresponding gain graph is then obtained as $W - \delta I$. By construction, such gain graphs have distinct eigenvalues $-\delta \pm \sqrt{k}$.

Below, we will mainly consider the generic case with $\delta = 0$. It should be noted that similar considerations are possible when $\delta \neq 0$, although these cases are considerably more restrictive. Indeed, if $\delta \neq 0$ then the adjacency matrix $A = W - \delta I$ satisfies $A^2 = -2\delta A + (k-1)I$, where $W^2 = kI$, and thus $4k$ must be a perfect square, by Lemma 7.1. (Note that A has degree $k-1$.) An example of such a case is the complete graph K_4, whose adjacency matrix A is related to the graphical Hadamard matrix $A - I$.

Another interesting link to the field of weighing matrices appears when one restricts oneself to the class of bipartite gain graphs. Indeed, if Ψ is bipartite, then its gain matrix A may be written as

$$A = \begin{bmatrix} O & B \\ B^* & O \end{bmatrix}, \tag{7.2}$$

and thus[1]

$$A^2 = \begin{bmatrix} BB^* & O \\ O & B^*B \end{bmatrix} = kI \iff BB^* = B^*B = kI.$$

That is, Ψ has exactly two distinct eigenvalues if and only if B is a square weighing matrix of weight k. In our below classification, we will will denote the bipartite gain graph obtained from a weighing matrix B as in (7.2) by $IG(B)$.

We have to place a note of care here. It follows easily that the direct sum of any two weighing matrices of equal weight is again a weighing matrix. However, by the same token, if W is the disjoint union of W' and W'', then $IG(W)$ is disconnected. Since we assume connectedness throughout, we require that W is irreducible.

The smallest nontrivial examples of unit weighing matrices are

$$W_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \; W_3 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & \varphi & \overline{\varphi} \\ 1 & \overline{\varphi} & \varphi \end{bmatrix} \text{ and } W_4.$$

In fact, we may draw some additional conclusions, regarding on these matrices.

Proposition 7.4. *Let Ψ be a connected, order-n gain graph with eigenvalues $\pm\sqrt{2}$. Then Ψ is switching isomorphic to $IG(W_2)$.*

Proof. Immediate from [8, Thm. 10], since any irreducible weighing matrix of weight 2 is equivalent to W_2. □

Using the subsequent result from Best et al. [8] that characterizes weighing matrices of weight 3, one also readily finds the following, analogous result.

Proposition 7.5. *Let Ψ be a connected, order-n gain graph with eigenvalues $\pm\sqrt{3}$. Then Ψ is switching isomorphic to either W_4, $IG(W_3)$ or $IG(W_4)$.*

[1] Note that $a = 0$ follows since bipartite gain graphs have symmetric spectra.

In fact, it turns out that these graphs (and K_4) are the only two-eigenvalue gain graphs with degree 3; this is shown formally in Section 7.6. Further examples of weighing matrices include

$$W_5 = CM\left(\begin{bmatrix}0 & 1 & \varphi & \varphi & 1\end{bmatrix}\right) \text{ and } W_7 = CM\left(\begin{bmatrix}-1 & 1 & 1 & 0 & 1 & 0 & 0\end{bmatrix}\right).$$

Of course, many more examples of weighing matrices may be (and have been) constructed, though we will not explicitly list them here. Several methods to generate such examples are discussed in the next section.

It should be noted that cubelike graphs, in particular, may often be equipped with a gain function such that the corresponding gain matrix is a weighing matrix. For example, $IG(W_4)$ is (switching equivalent to) a signed cube and by taking Kronecker products of the 2×2 Pauli matrices, Alon and Zheng [2] construct such gain graphs on graphs that may be obtained as a Cartesian product of a folded cube and a cube.

7.3.2 Recursive constructions

In the previous section, we have seen a construction that takes a given weighing matrix, and turns it into a gain graph with exactly two eigenvalues. In fact, if such a weighing matrix W has a zero diagonal, such that it characterizes a gain graph Ψ, then $IG(W)$ in a sense doubles Ψ. The following was effectively proven above, below (7.2).

Lemma 7.6. *Let Ψ be an order-n gain graph with exactly two eigenvalues $\pm\sqrt{k}$. Then $IG(\Psi)$ has order $2n$ and eigenvalues $\pm\sqrt{k}$.*

One might wonder whether the reverse also holds, when the trivial counterexamples such as W_2 and W_3 are excluded. This is not true, as is shown in the example below.[2]

Example 7.2. *Let B be the matrix defined as*

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

[2]Note that B is equivalent to W_4 under the operations listed in [8]. However, B is not graphical, while W_4 is.

Then the signed cube $IG(B)$ has eigenvalues $\pm\sqrt{3}$, while B itself is not graphical.

Many such examples may be constructed, by using a set of operations that map a given weighing matrix to another, which does not necessarily preserve the Hermitian property, or the zero diagonal. These operations include permuting the rows (eq. columns) or multiplying a row (eq. column) by a number in $\mathbb{T}$; see [8] for details.

An idea similar to the doubling operation above was recently used by Huang [65] in his proof of the Sensitivity Conjecture of Nisan and Szegedy on Boolean functions. For a given Hermitian matrix W with exactly two distinct eigenvalues $\pm\sqrt{k}$, one easily finds that

$$A = \begin{bmatrix} W & I \\ I & -W \end{bmatrix} \tag{7.3}$$

has distinct eigenvalues $\pm\sqrt{k+1}$. In particular, this construction was used by Huang to construct signed n-cubes; see [6] for more info. We will call this construction Huang's Negative Double, denoted $ND(\Psi)$.

Stanić [100] observed that under the same conditions, Sylvester's recursive construction for Hadamard matrices carries over to the current paradigm. That is, the matrix

$$B = \begin{bmatrix} W & W \\ W & -W \end{bmatrix} \tag{7.4}$$

also has two distinct eigenvalues, i.e., $\pm\sqrt{2k}$. This construction is, in turn, called the Sylvester Double and denoted $SD(\Psi)$. Moreover, we obtain variation on the above by adding an identity component to the off-diagonal blocks. Specifically, the matrix

$$B = \begin{bmatrix} W & W + iI \\ W - iI & -W \end{bmatrix} \tag{7.5}$$

has eigenvalues $\pm\sqrt{2k+1}$. This operation will be denoted $SD^*(\Psi)$, hereafter. Since these constructions are all applicable to graphical weighing matrices, the following should be clear.

Lemma 7.7. *Let Ψ be an order-n gain graph with distinct eigenvalues $\pm\sqrt{k}$. Then the distinct eigenvalues of $ND(\Psi)$ are $\pm\sqrt{k+1}$ and the distinct eigenvalues of $SD(\Psi)$ are $\pm\sqrt{2k}$. Finally, the distinct eigenvalues of $SD^*(\Psi)$ are $\pm\sqrt{2k+1}$.*

A final construction that follows a similar pattern was provided by Greaves [45] in his classification of cyclotomic matrices over the Gaussian and Eisenstein integers.

A concrete description of these is as as follows. Let C be an order-t weighing matrix with weight 1 and a zero diagonal, such that $C + C^*$ is also a unimodular matrix. Then, construct A as

$$A = \begin{bmatrix} C + C^* & C - C^* \\ C^* - C & -C - C^* \end{bmatrix}. \tag{7.6}$$

One is easily convinced that $A^2 = 4I$, and thus A has eigenvalues ± 2.

Note that $C + C^*$ is the gain matrix of a cycle with gain x, for some $x \in \mathbb{T}$. Using Proposition 4.4, we may without loss of generality switch such that all but one entry of C equal one, such that the final entry equals x. For C defined in such a way, and A obtained from C as in (7.6), we say that A is the gain matrix of a *toral tesselation* graph [45], which is denoted $T_{2t}^{(x)}$. Note that the graphs $T_{2t}^{(x)}$, $T_{2t}^{(\overline{x})}$, $T_{2t}^{(-x)}$, and $T_{2t}^{(-\overline{x})}$ are all switching isomorphic.

Finally, we note that a variation on (7.6) similar to (7.5) is also possible. That is,

$$B = \begin{bmatrix} C + C^* & C - C^* + I \\ C^* - C + I & -C - C^* \end{bmatrix},$$

which is later said to be a donut graph, has eigenvalues $\pm\sqrt{5}$. We discuss this construction in more detail in Section 7.6.4, when we use it to construct infinite families of gain graphs with eigenvalues $\pm\sqrt{5}$, for every even $n \geq 8$.

To end this section, the author would like to express some interest in similar recursive constructions that do not require its blocks to be weighing matrices. In particular, it seems plausible that gain graphs with two distinct eigenvalues that do not sum to zero, may also be expanded into larger graphs that keep much of their structure, and thereby have exactly two distinct eigenvalues, as well. However, such constructions are unknown to the author, at the time of writing.

7.4 Relations to systems of lines

Interestingly, the matter at hand has various links to other well-studied fields that are more geometric and algebraic in nature. In particular, numerous topics that are all based on of a system of lines in complex space are naturally tied to the highly structured matrices that we are interested in. The connection between systems of lines and highly symmetric graphs has been explored before, most notably in the classification of graphs with least eigenvalue -2 by Cameron et al. [15], which was recently extended to signed graphs by Greaves et al. [46]. In this work, we explore a similar connection in a much more general setting.

In this section, we will touch on several interconnected research areas that are concerned with these peculiar systems of lines. These topics include (Tight) Frames [106], Mutually Unbiased Bases (MUB) [32] and Symmetric Informationally Complete Positive Operator-Valued Measurements (SIC-POVM) [41]. For now, we aim to survey the various links and their subtleties in relation to two-eigenvalue gain graphs. The obtained perspective is put to work in Section 7.5, where an algebraic approach is taken to characterize all two-eigenvalue gain graphs with small least multiplicity.

7.4.1 The Eisenstein matrix

In Chapter 4, we have considered a Hermitian adjacency matrix for Signed Directed Graphs. This matrix, which was called the Eisenstein matrix, after the group of unit Eisenstein integers $\mathbb{T}_6$ that make up its nonzero entries, may simply be considered to be the gain matrix of a gain graph. The current line of questioning does therefore apply. In this section, we will offer a brief intermezzo in which we will restrict the allowed edge gains to the entries of $\mathbb{T}_6$, in order to illustrate the perspective one might obtain by considering systems of lines.

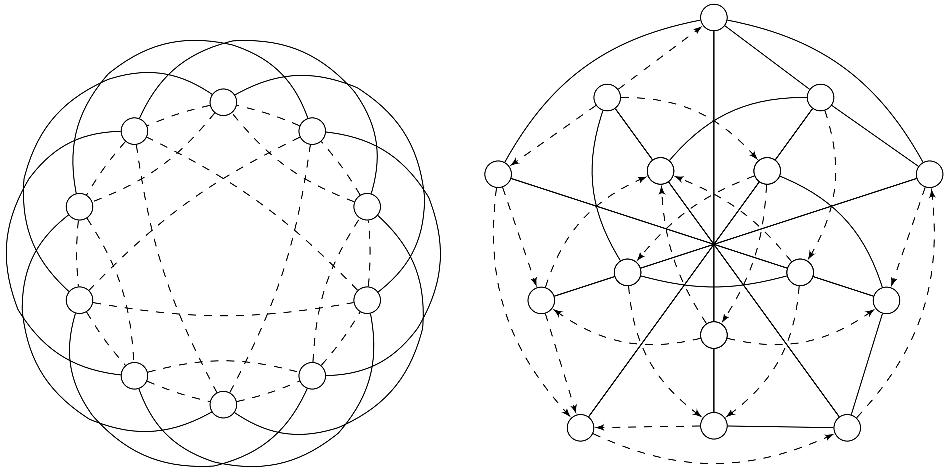
The attentive reader may have observed that almost all examples (excluding Example 1) have had either $a = 0$ or $a = k - 1$. (Recall that $a = \theta_1 + \theta_2$ and $k = -\theta_1\theta_2$, where k is the degree of the corresponding gain graph.) As an illustrative exercise, let us attempt to construct signed digraphs with exactly two distinct eigenvalues, such that $0 < a < k - 1$.

An important detail to note here, is that $a \in \mathbb{Z}$ when the edge gains are restricted to $\mathbb{T}_6$. Indeed, since $A^2 = aA + kI$, we have

$$a = \sum_h A_{ih}A_{hj}A_{ji}, \tag{7.7}$$

for some nonzero A_{ij}. In this particular case, (7.7) then means a is a sum of elements in $\mathbb{T}_6$. Moreover, since $a = \theta_1 + \theta_2$, a is real and it follows naturally that $a \in \mathbb{Z}$. Hence, Lemma 7.1 may be applied.[3] (As an aside, a parallel argument holds when the gains are restricted to $\mathbb{T}_4$.)

[3]The same conclusion can be reached by using that A has a characteristic polynomial with integer coefficients, see e.g. Theorem 1.2. It then follows that its minimal polynomial $\lambda^2 - a\lambda - k$ has integer coefficients, as well.



(a) **(b)**

Figure 7.2 – Signed digraphs with spectra $\left\{3^{[2n/5]}, -2^{[3n/5]}\right\}$. (In (b), all three vertices hit by each straight line through the center of the picture are pairwise adjacent; all such edges have gain 1.)

Since Lemma 7.1 applies, the tuple (a, k) must satisfy $a^2 + 4k = b^2$ for some integer b. One is easily convinced that the smallest value of k such that $0 < a < k-1$ and the above holds is $k = 6$, in which case $a = 1$. It then follows that $\theta_1 = 3$ and $\theta_2 = -2$, and thus $m = 2n/5$ and $n - m = 3n/5$. This, in turn, implies that n must be a multiple of 5. In the below, we will consider a number of possible values n, and discuss possible examples of signed digraphs with two distinct eigenvalues and the before mentioned parameters.

The smallest possible n is $n = 10$. Ramezani [89] has constructed a signed graph (gains in $\mathbb{T}_2 \subset \mathbb{T}_6$) with the above spectrum on the complement of the Petersen graph. Ramezani moreover shows that this example, illustrated in Figure 7.2a, is actually a member of an infinite family of signed graphs with two distinct eigenvalues on the triangular graphs[4] $\Delta(m)$.

The next case, $n = 15$, also admits an example with the above parameters that is related to the triangular graphs. Below, we propose a construction on the generalized quadrangle $GQ(2,2)$, which is the complement of $\Delta(6)$, and illustrated in Figure 7.2b. To find the desired example, we employ the so-called hexacode [22]: a 3-dimensional linear code of length 6 over $GF(4) = \{0, 1, \varphi, \overline{\varphi}\}$, where φ and $\overline{\varphi}$ denote the third

[4]The triangular graph $\Delta(m)$ is the line graph of complete graph K_m.

roots of unity. Specifically, the hexacode is defined by

$$H = \left\{ \begin{bmatrix} p_2 & p_1 & p_0 & f(1) & f(\varphi) & f(\overline{\varphi}) \end{bmatrix} \; : \; f(x) = p_2 x^2 + p_1 x + p_0, \; p_j \in GF(4) \right\}.$$

In particular, the hexacode has 45 elements, called codewords, of weight 4, occurring in 15 1-dimensional subspaces; i.e., lines through the origin. From each such subspace, we choose one nonzero codeword which we consider as a vector in $\mathbb{C}^6$. These vectors $v_h, h \in [15]$, represent our vertex set. It is easily verified that each of the possible 15 supports occurs exactly once, and distinct supports can intersect in 2 or 3 positions. Moreover, the construction is such that if two codewords v_h and v_j have supports that intersect in 3 positions, then the corresponding inner product is always $v_h^* v_j = 1 + \varphi + \overline{\varphi} = 0$. If two codewords have supports that intersect in 2 positions, then the inner product is either $1 + 1$, $\varphi + \varphi$, or $\overline{\varphi} + \overline{\varphi}$. Hence, we may define an Eisenstein matrix $\mathcal{E}$ (gain matrix) by

$$\mathcal{E}_{hj} = \frac{1}{2} v_h^* v_j, \; h \neq j; \mathcal{E}_{jj} = 0.$$

Note that the above indeed defines a signed directed graph, since $\mathcal{E}_{hj} \in \{0, 1, \varphi, \overline{\varphi}\}$ and $\mathcal{E}$ is Hermitian. Moreover, if we set M to be the matrix whose columns are the v_j, then according to the definition above $\mathcal{E} = \frac{1}{2} M^* M - 2I$, and thus

$$\mathcal{E}^2 = \frac{1}{4} M^* M M^* M - 2M^* M + 4I = \frac{1}{2} M^* M + 4I = \mathcal{E} + 6I, \tag{7.8}$$

where the second equality follows since $MM^* = 10I$. (A similar fact should hold in general; this is formalized in Proposition 7.8, below.) Lastly, note that by (7.8), it follows that $\mathcal{E}$ indeed has the desired spectrum $\{3^{[6]}, -2^{[9]}\}$.

Note that, by definition, taking a different representative vector of a subspace will lead to a signed digraph that is switching equivalent with the original one. The corresponding equivalence class is, in fact, the only one with the desired spectrum with this particular underlying graph, thus yielding an easy spectral characterization. The particulars to this fact are quite tedious, and have been verified by computer.

The construction above has some ties to previously studied objects. It is, for example, closely related to the so-called tilde-geometry [88]. Moreover, Figure 7.2b is in a sense a quotient of the distance-regular antipodal 3-cover of the collinearity graph of the generalized quadrangle of order 2 [13, p. 398]. This, in turn, is a distance-regular graph that is defined on the above mentioned 45 codewords of weight 4, with adjacency of vertices h and j if $\mathcal{E}_{hj} = \frac{1}{2}v_h^* v_j$ equals 1.

Most importantly, the above discussion sheds some light on the way in which systems of lines (1-dimensional subspaces) are connected to the remarkable gain graphs that are the topic of this work. In essence, one needs systems of lines that are either orthogonal to one-another, or are all separated by the same specific angle. Correspondingly, Ramezani's examples on $\Delta(m)$ can be described by the lines through the vectors $e_h - e_j$ $(h < j)$ in $\mathbb{R}^m$, where e_h is a standard basis vector. Systems of lines that are pairwise separated by the same angle (so-called *equiangular* lines) will be of special interest, later in this section. First, we offer a little more general insight based on the above.

7.4.2 Decomposition as a $\{0, \alpha\}$-set

In the above, we have showcased a clear parallel between gain graphs with few distinct eigenvalues, and systems of lines that are separated by few distinct angles. The equation $\mathcal{E} = \frac{1}{2}M^*M - 2I$ is particularly reminiscent of a Gram matrix, though it does need a little additional work.

In general, if $A := A(\Psi)$ for some gain graph Ψ with smallest eigenvalue $\theta_{\min}$, whose multiplicity is $n - m$, then $I - \theta_{\min}^{-1}A$ is a positive semi-definite matrix with rank m. It can therefore be represented as the Gram matrix of (Hermitian) inner products of a set of n unit vectors $\{u_1, u_2, \ldots, u_n\}$ in complex space $\mathbb{C}^m$. As before, the absolute values $|u_i^* u_j|$ of these inner products represent the angles between the lines through the unit vectors. In our case, there are exactly 1 or 2 such angles. Correspondingly, the inner product of every two distinct unit vectors has absolute value either zero or $-\theta_{\min}^{-1}$. In the study of lines in (complex) space, this phenomenon is known as a $\{0, \alpha\}$-set, where $\alpha = -\theta_{\min}^{-1}$ is the non-orthogonal separation angle.

Example 7.3. *Recall* $W_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ *and let* $\Psi = IG(W_2)$. *Then* Ψ *has eigenvalues* $\pm\sqrt{2}$, *and thus*

$$I - \theta_2^{-1}A(\Psi) = \begin{bmatrix} 1 & 0 & \frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \\ 0 & 1 & \frac{1}{2}\sqrt{2} & -\frac{1}{2}\sqrt{2} \\ \frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} & 1 & 0 \\ \frac{1}{2}\sqrt{2} & -\frac{1}{2}\sqrt{2} & 0 & 1 \end{bmatrix},$$

which is the Gram matrix of the unit vectors

$$u_1 = \begin{bmatrix}1 & 0\end{bmatrix}^\top, \quad u_2 = \begin{bmatrix}0 & 1\end{bmatrix}^\top, \quad u_3 = \frac{1}{2}\sqrt{2}\begin{bmatrix}1 & 1\end{bmatrix}^\top, \quad u_4 = \frac{1}{2}\sqrt{2}\begin{bmatrix}1 & -1\end{bmatrix}^\top.$$

As before, the vector notation can be translated to a matrix (outer)product. Let N be the matrix whose columns are the vectors $u_1, \dots, u_n$. Then, by the above, $N^*N = I - \theta_{\min}^{-1}A$. However, one cannot carelessly expect that any $\{0, \alpha\}$-set of unit vectors will yield a two-eigenvalue gain graph, as is showcased in the following example.

Example 7.4. *Let $\{u_1, \dots, u_4\}$ be the collection of vectors*

$$\left\{\begin{bmatrix}1 & 0 & 0\end{bmatrix}^\top, \begin{bmatrix}\frac{1}{2} & \frac{1}{2}\sqrt{3} & 0\end{bmatrix}^\top, \begin{bmatrix}0 & \frac{1}{3}\sqrt{3} & \frac{1}{3}\sqrt{6}\end{bmatrix}^\top, \begin{bmatrix}\frac{1}{2} & -\frac{1}{6}\sqrt{3} & \frac{1}{3}\sqrt{6}\end{bmatrix}^\top\right\}$$

and let $N = \begin{bmatrix}u_1 & u_2 & u_3 & u_4\end{bmatrix}$. Then

$$N^*N = \frac{1}{2}\begin{bmatrix}2 & 1 & 0 & 1\\ 1 & 2 & 1 & 0\\ 0 & 1 & 2 & 1\\ 1 & 0 & 1 & 2\end{bmatrix} = I - (-2)^{-1}A(C_4),$$

where C_4 is the undirected four-cycle, which has spectrum $\{-2, 0^{[2]}, 2\}$.

This goes to show that n unit vectors that are separated by one of two angles do not, in general, suffice to find a two-eigenvalue gain graph. However, the following interesting fact gives us an easy characterization.

Proposition 7.8. *Let A be an order-n Hermitian matrix with least eigenvalue $\theta_{min} \neq 0$, whose multiplicity is $n - m$, $m > 0$, and let $N \in \mathbb{C}^{m\times n}$ be such that $N^*N = I_n - \theta_{min}^{-1}A$. Then A has exactly two distinct eigenvalues if and only if $NN^* = zI_m$ for some $z \in \mathbb{R}$.*

Proof. A has exactly two distinct eigenvalues if and only if $N^*N \in \mathbb{C}^{n\times n}$ has a spectrum given by $\left\{0^{[n-m]}, 1 - \theta_2^{-1}\theta_1^{[m]}\right\}$. Since N^*N and NN^* coincide on the nonzero eigenvalues, this is equivalent with $NN^* \in \mathbb{C}^{m\times m}$ having a single eigenvalue $1 - \theta_1\theta_2^{-1}$ with multiplicity m. This, in turn, occurs if and only if $NN^* = (1 - \theta_1\theta_2^{-1})I$. □

It should be noted that if A has a zero diagonal and constant-norm nonzero entries, then $z = 1 - \theta_1\theta_2^{-1} = n/m \in \mathbb{Q}$. Furthermore, if the columns of N form a $\{0, \alpha\}$-set of unit vectors such that $NN^* = zI$, then either $N^*N = I$ and the columns of N form an orthonormal basis ($z = 1$, $n = m$, and the matrix $A = 0$), or $N^*N = I + \alpha A$ and A is a two-eigenvalue gain graph.

To conclude this section, we touch on some interesting facts. In case two of the unit vectors from $u_1, u_2, \ldots, u_n$ are scalar multiples of each other, then their inner product is a unit. This implies that $\theta_{\min} = -1$ and therefore that the corresponding unit gain graph is switching isomorphic to a complete graph. It follows that $m = 1$ and the u_j are simply unit complex numbers. This somewhat trivial case will be excluded in the classifications discussed in Section 7.6.

Moreover, one should also exercise some care when taking induced subgraphs. Instinctively one might be keen to claim that taking a subset of a given system of lines that constitutes a two-eigenvalue gain graph will yield another one. However, one cannot carelessly remove columns from N without affecting the entries of NN^*, the latter of which must be a multiple of the identity. In Section 7.5.2, we will discuss a method to obtain two-eigenvalue subgraphs.

7.4.3 Bounds

An intuitive question related to the matter of lines in complex space has to do with existence. Specifically: how many lines can there be in an m dimensional space, such that the angle between each pair is one of a given number of possible angles. In general, the classic result by Delsarte et al. [31], that bounds the number n of distinct lines in $\mathbb{C}^m$, whose separation angles are all contained in some collection $\mathcal{A}_s = \{\alpha_1, \alpha_2, \ldots, \alpha_s\}$ tells us that

$$n \leq \binom{m+s-1}{m-1}\binom{m+s-1-\varepsilon}{m-1}, \tag{7.9}$$

where $\varepsilon = 1$ if $0 \in \mathcal{A}_s$ and zero otherwise. This has been called the absolute bound for systems of lines; for a particularly concise proof, the interested reader is referred to [70]. As should be evident from the previous section, we will exclusively concern ourselves with the cases $\mathcal{A}_1 = \{\alpha\}$ and $\mathcal{A}_2 = \{0, \alpha\}$, for $\alpha \in (0, 1)$. In these cases, (7.9) reduces to $n \leq m^2$ and $n \leq \frac{1}{2}m^2(m+1)$, respectively. However, the latter bound may be sharpened under particular circumstances.

Proposition 7.9. *Let Ψ be an order-n gain graph with spectrum $\{\theta_1^{[m]}, \theta_2^{[n-m]}\}$, such that $\Gamma(\Psi)$ has degree k and an eigenvalue $-\frac{km}{n-m}$ with multiplicity $m' \geq 0$. Then $n \leq m^2 + m'$.*

Proof. Let $\{v_j\}_{j=1}^n$ be the corresponding system of vectors in $\mathbb{C}^m$, and consider the matrix M defined by $M_{hj} = \operatorname{Tr}(v)_h\, v_h^* v_j v_j^* = |v_h^* v_j|^2$. Then $M = I + \frac{n-m}{km}B$, where B is the adjacency matrix of $\Gamma(\Psi)$. Consider now the linear transformation $T : \mathbb{C}^n \mapsto \mathbb{C}^{m\times m}$ defined by $T(x) = \sum_j x_j v_j v_j^*$. Then, by the rank-nullity theorem, one has $n = \dim \operatorname{Range}(T) + \dim \ker(T) \leq m^2 + m'$. Here, it is used that $\dim \ker(T) \leq m'$ since $T(x) = 0$ implies $Mx = 0$ and thus x is in the eigenspace of B for eigenvalue $-\frac{km}{n-m}$. □

The above directly ties into some of the well-studied geometric objects that will be discussed shortly. For example, if $\Gamma = K_{t\times m}$, then $m' = n/m - 1$ and the above reduces to $n \leq m(m+1)$. These are precisely the underlying graph and the bound that occur in the case of Mutually Unbiased Bases, which is treated in Section 7.4.6. Furthermore, it should be clear from the proof above that in the case of equality, the projectors $v_j v_j^*$ span $\mathbb{C}^{m\times m}$. If, additionally, $m' = 0$ then they form a basis of $\mathbb{C}^{m\times m}$. This corresponds to the absolute bound in the case of an $\mathcal{A}_1$-set, which is attained by a 'symmetric, informationally complete positive operator-valued measurement,' which are treated in Section 7.4.5.

To conclude this section, we touch on the relative bound, which originally was a bound on the eigenvalues of Seidel matrices by Van Lint and Seidel [75, Lemma 6.1]. It bounds the angle α of a system of n lines (represented by unit vectors u_j) in $\mathbb{C}^m$ with mutual angles at most α. Although this bound does not have any implications for our work, it is good to notice that equality in this bound leads to a two-eigenvalue graph. This is immediately clear from the proof[5] by Brouwer and Haemers [11, Prop. 10.6.3].

7.4.4 Tight frames

Another school of thought is concerned with the notion of *tight frames*. Boiled down to its essence, a tight frame is an over-complete collection of vectors that span some vector space; that is, the frame contains some deliberately redundant members. Under the right circumstances, this redundancy is actually an advantage. Since their

[5] Indeed, note that in the case of equality $\operatorname{Tr}(Y)\,Y^* = 0$ and thus $Y = \sum_j u_j u_j^* - \frac{n}{m}I = 0$, which implies that $\sum_j u_j u_j^*$, which in our notation is equal to NN^*, is a multiple of I, and hence Proposition 7.8 applies. Therefore, we indeed have equality if and only if the corresponding gain graph has two distinct eigenvalues.

conception, tight frames have found the most use in the development of *wavelets,* since decomposition into tight frames rather allowed for far simpler representation than orthonormal bases would.

Let us recall the formal definitions from [106]. Formally, a frame is a set of vectors $\{v_k\}_{k\in\mathcal{K}}$ in a Hilbert space $\mathcal{H}$, indexed by some collection $\mathcal{K}$, that satisfy

$$c_1\|u\|^2 \leq \sum_{k\in\mathcal{K}} |\langle u, v_k\rangle|^2 \leq c_2\|u\|^2 \quad \forall u \in \mathcal{H},$$

for some constants $0 < c_1 \leq c_2 < \infty$. In case $c_1 = c_2$, then $\{v_k\}_{k\in\mathcal{K}}$ is said to be a *tight frame.* Moreover, in case $c_1 = c_2 = 1$, then $u = \sum_{k\in\mathcal{K}}\langle u, v_k\rangle v_k$ for any $u \in \mathcal{H}$ and the set $\{v_k\}_{k\in\mathcal{K}}$ is called a *normalized tight frame.* In particular, note that c_1 is merely a scaling factor, when the frame is tight.

While there are definitely similarities to the typical bases that one is used to, there are some important differences. Most importantly, $\mathcal{K}$ can be arbitrarily much larger than $\dim\mathcal{H}$, and $\{v_k\}_{k\in\mathcal{K}}$ could even contain repeated vectors. In particular, the following theorem, which is in essence a special case of an old result known as Naimark's dilation theorem [26], has provided the author with considerable insight.

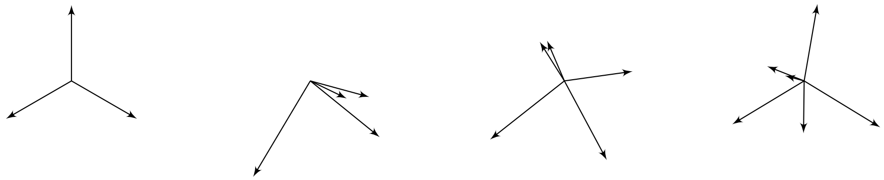
Theorem 7.10. *(Naimark) Every finite normalized tight frame $\{v_k\}_{k\in\mathcal{K}}$ for $\mathcal{H}$ is the orthogonal projection onto $\mathcal{H}$ of an orthonormal basis for a space of dimension $|\mathcal{K}|$, and vice versa.*

A clear parallel to our case becomes evident from the following characterization.

Proposition 7.11. *[106, Prop. 2.1] A finite sequence $\{v_k\}_{k\in\mathcal{K}}$ in $\mathcal{H}$ is a tight frame for $\mathcal{H}$ with frame bound c if and only if $NN^* = cI$. Here, N is the synthesis operator, i.e., $N(x) = \sum_{j=1}^{n} x_j v_j$ for $x \in \mathbb{C}^n$ and N^* is the (dual) analysis operator, i.e. $N^*(x)_j = \langle x, v_j\rangle$.*

Indeed, we observe a striking similarity to Proposition 7.8. We do not, however, immediately obtain equivalence. The main distinction between a general tight frame and the systems of lines that are of interest for this work, is that we require that the the frame vectors to have unit norm.

Note that indeed, this does not have do be the case, as is illustrated in Figure 7.3. Thus, we are, in fact, looking for a special case of the above, which are called *equal-norm* tight frames. In particular, by Propositions 7.11 and 7.8, it follows that $\{v_k\}_{k\in\mathcal{K}}$ is a unit-norm tight frame if and only if it corresponds to a two-eigenvalue gain graph via the usual construction.



(a) **(b)** **(c)** **(d)**

Figure 7.3 – Three tight frames in $\mathbb{R}^2$ of order $3, 4, 5, 6$, respectively. Only (a) is equal-norm.

The former case, in which the $\{v_k\}_{k\in\mathcal{K}}$ are an $\mathcal{A}_1$-set, is known as an *equiangular* tight frame. These have been studied quite extensively, see e.g. [103, 36, 35], and will translate nicely to a two-eigenvalue gain graph on a complete graph. In addition to various sporadic examples, some infinite families of equiangular tight frames have been uncovered. For example, the vectors

$$[0 \;\; \tau \;\; \sigma]^\top, \;\; [\sigma \;\; 0 \;\; \tau]^\top, \;\; [\tau z \;\; \sigma \;\; 0]^\top, \;\; [0 \;\; \tau \;\; -\sigma]^\top, \;\; [-\sigma \;\; 0 \;\; \tau]^\top, \;\; [\tau z \;\; -\sigma \;\; 0]^\top \tag{7.10}$$

form an equiangular tight frame for arbitrary $z \in \mathbb{T}$ if $\tau = \sqrt{\frac{5+\sqrt{5}}{10}}$, $\sigma = \sqrt{\frac{5-\sqrt{5}}{10}}$. Interestingly, the corresponding gain graph is, in fact, a donut graph (see Definition 7.1) with

$$C = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & \overline{z} & 0 \end{bmatrix}.$$

Moreover, in his article [93], Renes obtains an infinite family of equiangular tight frames of increasing order, based on the quadratic residues of prime powers of Gaussian primes (i.e., prime numbers congruent to 3 mod 4). Below, we showcase an infinite family of gain graphs that may be distilled from this construction.

Theorem 7.12. *[93] Let p be a Gaussian prime and let $n := p^z$, $z \in \mathbb{N}$. Then define the $n \times n$ matrix M by*

$$M_{jh} = \begin{cases} 0 & \text{if } j = h \\ 1 & \text{if } j \neq h \text{ and } h - j \text{ is a quadratic residue in } GF(n) \\ -1 & \text{otherwise.} \end{cases}$$

Now the matrix A, obtained from M as

$$A = (n+1)^{-1/2}\left(I - J - i\sqrt{n}M\right)$$

has exactly two distinct eigenvalues. Specifically, it has an eigenvalue $\sqrt{n+1}$ with multiplicity $(n-1)/2$ and an eigenvalue $-(n-1)/\sqrt{n+1}$ with multiplicity $(n+1)/2$.

Corollary 7.12.1. *For a given Gaussian prime p and $n = p^z$, $z \in \mathbb{N}$, the $n \times n$ matrix A as above defines a complex unit gain graph with exactly two distinct eigenvalues, whose underlying graph is K_n.*

In case the frame vectors are allowed to be either orthogonal, or separated by angle α, then much less previous work is readily available. Some work has been done on so-called 2-angle tight frames or two-distance tight frames: see e.g., [4]. However, their setting is more general (our case fixes one of the allowed angles to zero) and such works are generally concerned with constructions without orthogonal vectors.

7.4.5 SIC-POVM

As was briefly touched upon, an interesting link to two-eigenvalue gain graphs finds its origin in foundational quantum mechanics. In particular, one needs to be especially careful when measuring the state of a quantum algorithm. The foremost candidate to become the 'standard quantum measurement' is the so-called *symmetric, informationally complete, positive operator-valued measure* (SIC-POVM); a measure that is in possession of certain desirable qualities.

Slightly paraphrasing [41], an IC-POVM is described by m^2 positive semi-definite operators $\{E_j\}_{j=1}^{m^2}$ that span the m^2-dimensional space of observables on an m-dimensional Hilbert space $\mathcal{H}$. It is called an SIC-POVM if, in addition, it also satisfies the following three conditions:

1. E_j is rank one for all $j \in \{1, \ldots, m^2\}$,
2. $\mathrm{Tr} E_j E_h = c$ for all $j \neq h$, $j, h \in \{1, \ldots, m^2\}$,
3. $\mathrm{Tr} E_j = b$ for all $j \in \{1, \ldots, m^2\}$,

where b and c are nonnegative constants. In the below, we choose $b = 1$ without loss of generality.

There is a clear relation of the above to an $\mathcal{A}_1$-set of lines that attains the bound in (7.9). Specifically, the above is equivalent to a system of m^2 unit-norm vectors in an m-dimensional complex space, with pairwise equal inner products, in absolute value. It is well-known that this system is, in fact, an equiangular tight frame, whose vectors all have unit-length. Thus, it corresponds to a two-eigenvalue gain graph in the usual way.

Lemma 7.13. *Let $\{E_1, E_2, \ldots, E_n\}$ be a SIC-POVM in $\mathbb{C}^m$, so $n = m^2$. Let N be the matrix whose columns are $v_1, v_2, \ldots, v_n$, where $E_j = v_j v_j^*$ for every $j \in [n]$. Then $A = \sqrt{m+1}(N^*N - I)$ is the gain matrix of a two-eigenvalue gain graph.*

The simplest example of a nontrivial SIC-POVM is obtained in $\mathbb{C}^2$ by the vectors that form the vectices of a regular tetrahedron in the Bloch sphere. Specifically, let

$$N_2 = \frac{1}{\sqrt{3}} \begin{bmatrix} \sqrt{3} & 1 & 1 & 1 \\ 0 & \sqrt{2} & \sqrt{2}\varphi & \sqrt{2}\varphi^2 \end{bmatrix}, \tag{7.11}$$

then $A(\Psi) = \sqrt{3}(N_2^* N_2 - I) = W_4$, which as we know has eigenvalues $\pm\sqrt{3}$.

The first example that has not appeared in this work yet is obtained from a SIC-POVM of dimension 3, is given by columns of the matrix N_3, below. (Recall that $\omega = (1 + i\sqrt{3})/2$.)

$$N_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & \omega & 1 & 0 & -1 & 1 & 0 & \overline{\omega} \\ \omega & 1 & 0 & -1 & 1 & 0 & \overline{\omega} & 1 & 0 \\ 0 & \omega & 1 & 0 & -1 & 1 & 0 & \overline{\omega} & 1 \end{bmatrix} \tag{7.12}$$

Given the results we have seen so far, the reverse construction is straightforward, though one would need a gain graph with very particular properties to work with.

Proposition 7.14. *Let $\Psi = (K_n, \psi)$ be a gain graph of order $n = m^2$, for some $m \in \mathbb{N}$, whose spectrum is*

$$\Sigma_\Psi = \left\{ (m-1)\sqrt{m+1}^{[m]}, -\sqrt{m+1}^{[m^2-m]} \right\}.$$

Then there exists an $N \in \mathbb{C}^{m \times n}$ such that $N^*N = I + \frac{1}{\sqrt{m+1}} A(\Psi)$; the columns of N correspond to a SIC-POVM of dimension m.

An interesting application of the above could be the search for new SIC-POVMs through the search for their corresponding gain graphs. As of yet, we do not posses the means to find such graphs, though further development of constructions such as the ones in Section 7.3 might lead to surprising results on this front.

7.4.6 Mutually Unbiased Bases

Another relevant concept from quantum information theory is that of *Mutually Unbiased Bases* [32]. Where a SIC-POVM is effectively a maximum $\mathcal{A}_1$-set, a collection of MUBs is a particular $\mathcal{A}_2$-set. Formally, two orthonormal bases $\{e_j\}_{j=1}^m$ and $\{f_h\}_{h=1}^m$ of $\mathbb{C}^m$ are said to be mutually unbiased if $|e_j^* f_h|^2 = 1/m$ for all $j, h \in [m]$.

Much is known about MUBs. For instance, the maximum number of MUBs in $\mathbb{C}^m$ is $m+1$ when m is a prime power, i.e., $m = p^z$, $z \in \mathbb{N}$, with p prime. Yet, if m is a different composite number, then the maximum number of MUBs is not known; even relatively small cases such as $m = 6$ remain open[6].

From the definition, one may already have observed the clear parallel to two-eigenvalue gain graphs. Indeed, if N is the $m \times (t \cdot m)$ matrix whose columns are t MUBs, then $A = \sqrt{m}(N^*N - I)$ defines a unit gain graph. Moreover, it follows from the definition that $NN^* = tI$, and thus Proposition 7.8 applies, confirming that A has exactly two distint eigenvalues $(t-1)\sqrt{m}$ and $-\sqrt{m}$. Note that its underlying graph is the complete multipartite graph $K_{t\times m}$.

We will briefly discuss some examples. For the smallest nontrivial case, the standard basis and the 4 vectors

$$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i^j \end{bmatrix}, j \in \{0, 1, 2, 3\},$$

together form 3 MUBs in $\mathbb{C}^2$. The corresponding two-eigenvalue gain graph, hereafter indicated by $K_{2,2,2}^{(\gamma)}$, is described by the following matrix:

$$A(K_{2,2,2}^{(\gamma)}) = \begin{bmatrix} 0 & 0 & -i & i & 1 & 1 \\ 0 & 0 & 1 & 1 & -1 & 1 \\ i & 1 & 0 & 0 & -\bar{\gamma} & \gamma \\ -i & 1 & 0 & 0 & -\gamma & \bar{\gamma} \\ 1 & -1 & -\gamma & -\bar{\gamma} & 0 & 0 \\ 1 & 1 & \bar{\gamma} & \gamma & 0 & 0 \end{bmatrix}, \tag{7.13}$$

[6] The general belief is that the maximum number of MUBs in $\mathbb{C}^6$ is 3.

where $\gamma = (1+i)/\sqrt{2}$. In similar fashion, one may take consider $\mathbb{C}^3$. Here, the vectors

$$\begin{bmatrix}1 & 0 & 0\end{bmatrix}^\top, \begin{bmatrix}0 & 1 & 0\end{bmatrix}^\top, \begin{bmatrix}0 & 0 & 1\end{bmatrix}^\top \text{ and } \frac{1}{\sqrt{3}}\begin{bmatrix}1 & \varphi^j & \varphi^h\end{bmatrix}^\top, \text{ where } j,h \in \{0,1,2\}, \tag{7.14}$$

form 4 MUBs in $\mathbb{C}^3$.

It should be clear that when the set of MUBs does not attain the upper bound $m+1$ on its size, the above still holds true. For example, the toral tesselation graph $T_8^{(x)}$, where $x \in \mathbb{T}$, may alternatively be obtained from a pair of MUBs in $\mathbb{C}^4$. Specifically, if N is the matrix whose columns are the standard basis appended with the basis formed by the vectors

$$\frac{1}{2}[1\ 1\ 1\ -1]^\top, \frac{1}{2}[1\ 1\ -1\ 1]^\top, \frac{1}{2}[1\ -1\ x\ x]^\top, \frac{1}{2}[-1\ 1\ x\ x]^\top,$$

the graph characterized by $2(N^*N - I)$ is switching isomorphic to $T_8^{(x)}$.

As with the SIC-POVMs in the previous section, the relation between gain graphs with two specific eigenvalues and MUBs is an equivalence.

Proposition 7.15. *Let Ψ be a gain graph on $K_{t\times m}$, with exactly two distinct eigenvalues $-\sqrt{m}$ and $(t-1)\sqrt{m}$. Then there exists an $N \in \mathbb{C}^{m\times tm}$ such that $A(\Psi) = \sqrt{m}(N^*N - I)$; the columns of N form t mutually unbiased bases in $\mathbb{C}^m$.*

7.5 A classification based on multiplicities

The previous section has mostly been concerned with drawing various parallels between the here considered gain graphs and various notions related to systems of lines in complex space. Existence of such systems, especially those whose cardinality is high compared to the dimension of the space in which they exist, is certainly no trivial issue. In turn, said dimension corresponds to the multiplicity of the largest eigenvalue of our gain graphs. As a consequence, we may use the discussed results to classify two-eigenvalue gain graphs with low multiplicity, by considering the systems of lines in low-dimension spaces.

This section first sets out to classify all two-eigenvalue gain graphs with least multiplicity at most 3. The remainder of the section is concerned with larger examples obtained from the Witting polytope, the Coxeter-Todd lattice, and a complex reflection group by Shepard and Todd. Additionally, we discuss the partitioning of their fundamental line sets into subsets which each constitute their own two-eigenvalue gain

m	Graph	Order	k	DS
1	K_n	n	$n-1$	*
	$IG(W_2)$	4	2	*
2	W_4	4	3	*
	$K_{2,2,2}^{(\gamma)}$	6	4	*
	2 MUBs from (7.14)	6	3	*
	$T_6^{(x)}$	6	4	
	Equation (7.10)	6	5	
3	Theorem 4.4	7	6	*
	3 MUBs from (7.14)	9	6	*
	Equation (7.12)	9	8	*
	4 MUBs from (7.14)	12	9	*

Table 7.1 – Classification of all two-eigenvalue gain graphs with least multiplicity at most 3. A star in the DS column indicates that any connected, cospectral gain graph is switching isomorphic.

subgraph.

7.5.1 Algebraic classification

Through careful evaluation of the available knowledge on the existence of the discussed systems of lines in low-dimensional spaces, we arrive at the complete classification presented in Theorem 7.16. Named graphs are listed as such; unnamed examples are referenced using the equation that contains it or an equivalent system of lines.

Theorem 7.16. *All two-eigenvalue gain graphs with least multiplicity at most* 3 *are switching isomorphic to one of the gain graphs in Table 7.1.*

The remainder of this section will systematically evaluate the various possible parameter choices to arrive at the classification presented above. An interesting fact, known as the Cvetković bound, is a particularly useful tool in the approach that is taken below.

Lemma 7.17. *[11, Thm. 3.5.1] Let* Ψ *be a gain graph with spectrum* $\left\{\theta_1^{[m]}, \theta_2^{[n-m]}\right\}$. *Then the largest coclique in* Ψ *has size at most* m.

Proof. Suppose Ψ contains a coclique of size $m+1$. Then, by eigenvalue interlacing, Ψ has $\lambda_{m+1} \geq 0$, which is a contradiction. $\square$

Recall that least multiplicity 1 occurs only for gain graphs that are switching equivalent to a complete graph, so we proceed to the smallest interesting case.

Multiplicity 2

Let us classify the gain graphs Ψ whose spectrum is exactly

$$\left\{\theta_1^{[m]}, \theta_2^{[n-m]}\right\}, \text{ where } m = 2. \tag{7.15}$$

As noted above, this corresponds to a system of lines in $\mathbb{C}^2$. Applying the bound in (7.9), we obtain that $n \leq 4$ if the gain graph is complete and $n \leq 6$ otherwise. In the former case, one trivially obtains K_3; the case $n = 4$ is exactly the unique SIC-POVM in (7.11), whose corresponding gain graph is[7] W_4. The non-complete case yields two more admissible gain graphs.

Lemma 7.18. *If Ψ is an order n gain graph with spectrum $\left\{\theta_1^{[2]}, \theta_2^{[n-2]}\right\}$ and degree $k < n-1$, then Ψ is switching isomorphic to either $IG(W_2)$ or $K_{2,2,2}^{(\gamma)}$.*

Proof. Since $k < n - 1$, Ψ corresponds to an $\mathcal{A}_2$-set. Without loss of generality, we choose the first vector to be the standard unit vector e_1. Then, since Ψ is not complete, at least one vector must be orthogonal to e_1, so (without loss of generality) we take the second unit vector e_2. Since we are working in $\mathbb{C}^2$, there is no vector that is orthogonal to both e_1 and e_2, so it follows that Ψ has (constant) degree $k = n - 2$. This, in turn, means that $\Gamma(\Psi)$ is complete multipartite $K_{t\times 2}$, and thus (by Proposition 7.15) Ψ corresponds to a pair ($n = 4$) or a set of three ($n = 6$) MUBs. This yields precisely a gain graph that is switching isomorphic to $IG(W_2)$ or to $K_{2,2,2}^{(\gamma)}$, respectively. □

Multiplicity 3

We may apply the same line of questioning for graphs with spectrum $\{\theta_1^{[3]}, \theta_2^{[n-3]}\}$. If $k = n - 1$, then the corresponding line system is an equiangular frame, and the absolute bound $n \leq 9$ applies. These have been classified in dimension 3 by Szöllősi [103], and the results are summarized in Table 7.2.

[7]Note that any unitary transformation of the system of lines does not change the corresponding gain graph. That is, if U is a unitary matrix, then $M := UN$ and N represent the same gain graph because $M^*M = N^*N$.

n	
3	Standard basis
4	Regular simplex
5	-
6	Corresponds to (7.10)
7	Corresponding graph obtained from Theorem 7.12
8	-
9	Corresponds to (7.12)

Table 7.2 – Classification $\mathcal{A}_1$-sets in $\mathbb{C}^3$ from Szöllősi [103], up to equivalence.

In case $k = n-2$, then $\Gamma(\Psi) = K_{t\times 2}$, where $t \geq 3$ since it was assumed throughout that $m \leq n/2$. In other words, the vectors come in orthogonal pairs, with vectors from distinct pairs being separated by some angle α. Note that for given n, m, and k, we may compute the value of θ_2, which, as discussed before, determines α. Furthermore, note that since $K_{t\times 2}$ does not have an eigenvalue $-3(2t-2)/(2t-3)$, Proposition 7.9 implies that $n \leq 9$. Using the above, we are left with just two cases: either $n = 6$ or $n = 8$. Let us first consider the former.

Lemma 7.19. *Suppose Ψ is a gain graph with spectrum $\{\theta_1^{[3]}, \theta_2^{[3]}\}$ and $k = 4$. Then $\Psi \sim T_6^z$ for some $z \in \mathbb{T}$.*

Proof. As before, $(n, m, k) = (6, 4, 3)$ implies that $\alpha = 1/2$. Since the vectors occur in orthogonal pairs, we may take the first two standard unit basis vectors as a starting point. Since vectors from distinct pairs must have an inner product equal to α in absolute value, it follows that any further candidate v is of the form $v = \begin{bmatrix} x/2 & y/2 & z/\sqrt{2} \end{bmatrix}^\top$, for $x, y, z \in \mathbb{T}$. It is not hard to see that the desired system is (up to equivalence) represented by the vectors

$$\begin{bmatrix}1\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\end{bmatrix}, \begin{bmatrix}1/2\\1/2\\1/\sqrt{2}\end{bmatrix}, \begin{bmatrix}1/2\\1/2\\-1/\sqrt{2}\end{bmatrix}, \begin{bmatrix}1/2\\-1/2\\z/\sqrt{2}\end{bmatrix}, \begin{bmatrix}1/2\\-1/2\\-z/\sqrt{2}\end{bmatrix} \tag{7.16}$$

for any $z \in \mathbb{T}$. Finally, note that the corresponding two-eigenvalue gain graph is indeed the order-6 toral tesselation graph $T_6^{(z)}$. (See the end of Section 7.3.) ☐

What is left is the the case $n = 8$. We will formally show that $(n, m, k) = (8, 3, 6)$ does not yield any two-eigenvalue gain graphs.

Lemma 7.20. *There is no gain graph* Ψ *with spectrum* $\{\theta_1^{[3]}, \theta_2^{[5]}\}$ *and* $k = 6$.

Proof. Since $(n, m, k) = (8, 3, 6)$ it follows that $\alpha = \sqrt{5/18}$ and $\Gamma(\Psi) = K_{4\times 2}$. Hence, the corresponding line system contains four pairs (v_j, v_{j+1}), $j \in \{1, 3, 5, 7\}$, of orthogonal lines, such that any two lines from distinct pairs are separated by angle α. Without loss of generality, choose the first pair to be $(v_1, v_2) = (e_1, e_2)$. Then any other candidate is of the form

$$v_j = \begin{bmatrix} \alpha x_j & \alpha y_j & \beta z_j \end{bmatrix}^\top \text{ with } x_j, y_j, z_j \in \mathbb{T} \text{ for } j = 3, \ldots, 8 \text{ and where } \beta = \frac{2}{3}.$$

As before we may assume w.l.o.g. that $x_j = 1$ for all $j = 3, \ldots, 8$. Now, if N is the matrix whose columns are $v_1, \ldots, v_8$ and Ψ is a two-eigenvalue gain graph, then NN^* is a multiple of the identity. In other words, the rows of N are orthogonal. It follows straightforwardly that

$$\sum_{j=3}^{8} y_j = 0 \quad \text{and} \quad \sum_{j=3}^{8} z_j = 0. \tag{7.17}$$

Furthermore, let $y := \bar{y}_3 y_4$ and $z := \bar{z}_3 z_4$. Then $v_3^* v_4 = \alpha^2 + \alpha^2 y + \beta^2 z = 0$ if and only if $y = -1 - \beta^2 \alpha^{-2} z$. Since $|y| = |z| = 1$, z is on the intersection of two real-centered circles on the complex plane, and thus there is (at most) one conjugate pair of solutions for z. Suppose that $\tilde{z}$ is such a solution, and set $\tilde{y} = -1 - \beta^2 \alpha^{-2} \tilde{z}$. By symmetry, we also have[8] $\bar{y}_5 y_6 = \bar{y}_7 y_8 = \tilde{y}$ and $\bar{z}_5 z_6 = \bar{z}_7 z_8 = \tilde{z}$. Plugging this into (7.17) yields $\sum_{j=3}^{8} y_j = 0$ if and only if $y_3 + y_5 + y_7 = 0$, and similarly $z_3 + z_5 + z_7 = 0$. Here, it is used that $\tilde{y} \neq -1$, since this would contradict $|z| = 1$.

Finally, w.l.o.g. assume $y_3 = z_3 = 1$. Then the equations $|y_5| = |y_7| = 1$ and $y_5 + y_7 = -1$ must simultaneously hold, which implies $y_5 = \pm\varphi$ and $y_7 = \bar{y}_5$; similarly $z_5 = \pm\varphi$ and $z_7 = \bar{z}_5$. But now $|v_3^* v_5| = |\alpha^2 + \alpha^2 y_5 + \beta^2 z_5| \neq \alpha$, which is a contradiction. $\square$

Finally, in case $k \leq n - 3$, we find that Ψ must contain a coclique of order (at least) 3.

Lemma 7.21. *Let* Ψ *be an order-*n *gain graph with constant degree* $k \leq n - 3$, *and spectrum* $\left\{\theta_1^{[3]}, \theta_2^{[n-3]}\right\}$. *Then* Ψ *contains a coclique of order* 3.

Proof. We will be reasoning with the system of lines that corresponds to Ψ in the usual way. Suppose that Ψ does not contain a coclique of order 3 and let e_1 be the

[8] Up to conjugation, though since $\overline{y_5 y_6} = \bar{y}_6 y_5$, equality is assumed without loss of generality.

first standard unit vector. If $k \leq n-3$, then there are (at least) two vectors that are orthogonal to e_1. Moreover, said vectors may not be orthogonal to one another, since this would imply existence of an order-3 coclique. Hence, they must be separated by an angle $\alpha = \sqrt{(n-3)/(3k)}$. Without loss of generality, choose the second unit vector e_2 and $v = [0\ \alpha\ z]$, where $|z| = \sqrt{1-\alpha^2}$.

Now, we may repeat the argument, since, in addition to e_1, there is at least one more vector that is orthogonal to e_2. Furthermore, said vector must make an angle α with e_1. Without loss of generality, choose $w = [\alpha\ 0\ z']$, where $|z'| = \sqrt{1-\alpha^2}$. However, now $|v^*w| = |z^*z'| = 1-\alpha^2$, which implies $\alpha = 1-\alpha^2$, and thus $\alpha = (\sqrt{5}-1)/2$, which is a contradiction for all possible (n,k). □

Essentially, by using the symmetry in the argument above, it follows that any vertex in a two-eigenvalue gain graph Ψ with the desired spectrum is contained in an order-3 coclique. Then, it is not too hard to see that the inclusion of such an order-3 coclique implies that the corresponding line system consist of MUBs.

Lemma 7.22. *Let Ψ be a two-eigenvalue gain graph with least multiplicity* 3. *If Ψ contains an order-3 coclique then the usual corresponding line system consists of mutually unbiased bases.*

Proof. Consider the corresponding line system. Since Ψ contains a coclique of size 3, the system contains an orthonormal basis; without loss of generality, assume that it is the standard basis.

Now, suppose another vector v has first entry 0. By considering $|e_2^*v|$ and $|e_3^*v|$, which should both equal α, it follows that $\alpha = \sqrt{1/2}$. Moreover, it also follows that $k < n-3$, since there are 3 vectors that are orthogonal to e_1. (Specifically, e_2, e_3 and v.) Hence, there must be a third vector with second entry 0, which (by repeating the above) must satisfy $|e_1^*w| = |e_3^*w| = \alpha$. But now $|v^*w| = |(e_3^*v)(e_3^*w)| = 1/2 \neq \alpha$, which is a contradiction. Hence, no vectors other than the standard basis may have zero entries, and thus $k = n-3$. The conclusion now follows since every vertex is contained in a unique order-3 coclique. □

Since there exists a limited number of such mutually unbiased bases, the following observation completes the classification.

Corollary 7.22.1. *If Ψ is a gain graph with spectrum $\{\theta_1^{[3]}, \theta_2^{[n-3]}\}$ then Ψ is switching equivalent to a gain graph obtained from two, three or four of the mutually unbiased bases in* (7.14).

At this point, we have methodically considered all possible tuples (n, m, k) for $m = 1, 2, 3$ to gradually discuss all entries of Table 7.1 and conclusively prove that no further candidates exist. Naturally, one could choose to increase the multiplicity further and apply more or less the same arguments again; the final series of arguments (concerning $k \leq n - m$) in particular appears as if it would carry over with little to no issues. However, since we feel that such a discussion would provide little new insight, we choose to move on.

7.5.2 Dismantling two-eigenvalue gain graphs

As was noted before, one must exercise considerable care when taking subgraphs of two-eigenvalue gain graphs. While it may at a first glance look intuitive to simply take a subset of the corresponding system of lines, the problem is that such a subset does not, in general, satisfy the necessary equation $NN^* = zI$. However, a reliable way to obtain such subsystems is reminiscent of the dismantlability of certain association schemes [81, 71, 30].

Suppose that the m-dimensional complex unit vectors $\{v_j\}_{j=1}^n$ correspond to a two-eigenvalue gain graph in the usual way. Then the matrix N, whose columns are the v_j, satisfies $NN^* = zI$ for some $z \in \mathbb{R}$. Now, if the columns of N can be partitioned and concatenated into two matrices N_1 and N_2, where the former also constitutes a two-eigenvalue gain graph, then clearly $N_1N_1^* = yI$. However, since $NN^* = \sum_{j=1}^n v_j v_j^* = N_1N_1^* + N_2N_2^*$, it follows that $N_2N_2^* = (z - y)I$, and thus, per the discussion following Proposition 7.8, the N_2 either corresponds to an empty graph, or to a two-eigenvalue gain graph.

Clearly, the above may simply be repeated so long as one can find a subset of the vectors that satisfies the required equation. In particular, the $\{v_j\}_{j=1}^n$ may be partitioned into s subsets that each satisfy $N_iN_i^* = z_iI$, with $z_i \in \mathbb{R}$ and $i = 1, \dots, s$. Hence, every union of such subsets constructs a two-eigenvalue gain graph. Moreover, since every such gain graph is regular, the corresponding partition is an equitable one. The last conclusion, in particular, smells a lot like dismantlability. Formally, we obtain the following.

Theorem 7.23. *Let $s \geq 2$ and let Ψ be a two-eigenvalue gain graph with a multiplicity m on vertex set V. Let $V_i, i = 1, \dots, s$ be a partition of V. If the induced subgraph on V_i is either an m-coclique or a two-eigenvalue gain graph with a multiplicity m, for all $i = 1, \dots, s-1$, then for each nonempty subset $\mathcal{I}$ of $\{1, 2, \dots, s\}$, the induced subgraph* *on $\cup_{i\in\mathcal{I}}V_i$ is either an m-coclique or a two-eigenvalue gain graph with a multiplicity m.*

One may observe that the above generalizes the case of MUBs. Indeed, each basis in a collection of MUBs corresponds to an m-coclique, so it is clearly a special case of Theorem 7.23. While the correspondence to MUBs (i.e., spectrum $\{\theta_1^m, \theta_2^{n-m}\}$ on underlying graph $K_{m,n/m}$) offers a clear way to partition the vertices, it is not clear how one obtains a partition into m-cocliques and two-eigenvalue gain graphs, in general. Nevertheless, this still yields an abundance of two-eigenvalue subgraphs of two-eigenvalue gain graphs that correspond to highly symmetric geometries, such as those discussed in Section 7.5.3.

7.5.3 More examples from geometric objects

We conclude this section by showcasing a number of new two-eigenvalue gain graphs that arise from various other well-studied combinatorial objects. Inspired by the construction of the example on 15 vertices in Section 7.4.1, we offer several constructions that follow a similar pattern. The constructions presented below are essentially found by drawing $\{0, \alpha\}$-sets from highly symmetric geometric objects. Moreover, by observing that these $\{0, \alpha\}$-sets contain several orthonormal bases, the obtained constructions may be dismantled into several more two-eigenvalue subgraphs.

The Witting polytope

Real polytopes have been generalized to complex Hilbert spaces for quite some time. While precise definitions do not exist for the general case, the regular complex polytopes have been completely characterized by Coxeter. We forego the details, though it would be fair to say that these geometries are highly symmetric, which enables us to translate (parts of) them to the desired systems of lines.

Consider the Witting polytope [25] in $\mathbb{C}^4$. Its 240 vertices occur in 40 1-dimensional subspaces, which form an $\mathcal{A}_2$-set meeting the absolute bound. In particular, take the 4 standard basis vectors along with

$$\frac{1}{\sqrt{3}}\begin{bmatrix}1 & 0 & -\varphi^j & -\varphi^h\end{bmatrix}^\top, \frac{1}{\sqrt{3}}\begin{bmatrix}1 & -\varphi^j & 0 & \varphi^h\end{bmatrix}^\top, \frac{1}{\sqrt{3}}\begin{bmatrix}1 & \varphi^j & \varphi^h & 0\end{bmatrix}^\top, \text{ and}$$

$$\frac{1}{\sqrt{3}}\begin{bmatrix}0 & 1 & -\varphi^j & \varphi^h\end{bmatrix}^\top, \text{ with } j, h \in \{0, 1, 2\}.$$

Then the matrix N, whose columns are the vectors above, satisfies $NN^* = 10I$, so that Proposition 7.8 applies. Indeed, $A = \sqrt{3}(N^*N - I)$ characterizes an order-40 unit gain graph whose spectrum is $\left\{9\sqrt{3}^{[4]}, -\sqrt{3}^{[36]}\right\}$, and whose underlying graph is the complement of the symplectic generalized quadrangle of order 3.

Finally, note that the 40 vectors above may be partitioned into ten orthonormal bases, which form a spread in said quadrangle. Following the discussion in Section 7.5.2, one may use this partition to get two-eigenvalue gain graphs with spectrum $\left\{(t-1)\sqrt{3}^{[4]}, -\sqrt{3}^{[4(t-1)]}\right\}$, $t \in \{2, \ldots, 10\}$.

A rank-5 complex reflection group

In the same vein, one may draw on the collection of complex reflection groups and distill a unit gain graph from its hyperplanes of symmetry. In particular, we consider the group named ST33 in the (complete) classification by Shephard and Todd [98].

The desired collection of vectors may roughly be divided into two parts. The former part consists of all vectors obtained from

$$\frac{1}{\sqrt{2}}[1 \quad -\varphi^j \quad 0 \quad 0 \quad 0]^\top, j = 0, 1, 2,$$

by permuting the first four entries in all possible ways, such that the leftmost nonzero entry is[9] $1/\sqrt{2}$; this yields 18 vectors belonging to distinct hyperplanes in $\mathbb{C}^4$. The second part, containing the remaining 27 vectors, is described by

$$\frac{1}{\sqrt{6}}[1 \quad \varphi^{j_1} \quad \varphi^{j_2} \quad \varphi^{j_3} \quad \sqrt{2}\varphi^{-j_1-j_2-j_3}]^\top, \text{ where } j_1, j_2, j_3 \in \{1.2.3\}.$$

This yields a total of 45 unit vectors, whose pairwise inner products have absolute value either 0 or $\frac{1}{2}$, such that every vector is orthogonal to exactly 12 others. Thus, the matrix $A = 2(NN^* - I)$ characterizes a unit gain graph with spectrum $\left\{16^{[5]}, -2^{[40]}\right\}$.

Note that the underlying graph is the generalized quadrangle of order $(4, 2)$, which does not have a spread. However, we have found a partition of the vector set that contains six orthonormal bases; this corresponds to a partial spread. By considering unions of such bases and their complementary sets, we obtain induced subgraphs whose spectra are $\left\{2(t-1)^{[5]}, -2^{[5(t-1)]}\right\}$ for $t = 2, \ldots, 8$. Interestingly, the corresponding gain matrix has entries in $\mathbb{T}_6$, so it (and its induced subgraphs) could be

[9] Note that the vector obtained by interchanging the two nonzero entries is a member of the same hyperplane.

interpreted as a signed digraph.

The Coxeter-Todd lattice

Finally, we consider the famous Coxeter-Todd lattice in $\mathbb{C}^6$, which finds its origin in the hexacode, discussed at the start of this section. It has various equivalent descriptions [21], which give rise to different interesting two-eigenvalue gain (sub)graphs. In particular, these graphs attain the absolute bound (7.9) in terms of order n with respect to the multiplicity 6. The descriptions may be distinguished by their base[10].

In the 2-base, take all 15 projectively distinct hexacodewords of weight 4, and take all of their variations by multiplying at most 3 nonzero entries of every such codeword by -1. Scaling them down yields a collection of 120 distinct unit vectors, that may be appended with a standard unit basis of $\mathbb{C}^6$ to find 126 unit vectors whose pairwise inner products have absolute value either 0 or $\frac{1}{2}$. Thus, as before, we find a two-eigenvalue gain graph. Note, specifically, that the before-mentioned example on 15 vertices clearly occurs as an induced subgraph of this construction, as its corresponding system of lines is a subset of the 126 vectors required here.

In fact, the 126 vectors decompose into 21 orthogonal bases. This is easy to see, since the gain graph above has an order-126 underlying graph that is the complement of the strongly regular graph that appears in Brouwer and Van Maldeghem [12] as $NO_6^-(3)$. According to [12], the complement of $NO_6^-(3)$ has chromatic number 21, which implies that the desired decomposition exists. This, as before, yields two-eigenvalue gain subgraphs of order $6t$, for $t = 2, \dots, 21$.

One might also consider the 3-base parallel. Indeed, take the 45 vectors obtained from

$$[i\sqrt{3}\ \ -i\sqrt{3}\varphi^c\ 0\ 0\ 0\ 0]^\top, c \in [3]$$

by permuting its entries in such a way that the first nonzero entry is strictly imaginary, and append with the 81 vectors

$$[1\ \varphi^{j_1}\ \ \varphi^{j_2}\ \ \varphi^{j_3}\ \ \varphi^{j_4}\ \ \varphi^{-j_1-j_2-j_3-j_4}]^\top \text{ with } j_1, \dots, j_4 \in [3].$$

It is easily verified that the pairwise inner products of these 126 vectors have absolute value either 0 or 3, and thus the usual construction applies, after scaling.

[10]The lattice is said to be represented in the b-base if all absolute values of the pairwise inner products of the coordinate vectors are divisible by b, before scaling [21].

It should be noted that the collections of 45 and 81 vectors also construct two-eigenvalue gain graphs (with two-eigenvalue subgraphs), that are notably different from the subgraphs of order $6t$, above. In fact, the 81 vectors of weight 6 have yet another interesting link to other combinatorial objects constructed by Van Lint and Schrijver [74], such as their partial geometry. There is a clear correspondence of the above 81 vectors and the dual code of [74, Construction 2]. The different inner products (up to conjugation) of our vectors correspond to the weights in this dual code [74, Table III], and define a 4-class fusion scheme of the 8-class cyclotomic association scheme on $GF(81)$, which can be further fused to an amorphic association scheme [29]. We should note that Roy and Suda [95] have obtained many results such as the above, where the inner products give rise to various association schemes. These most interesting constructions are called spherical t-designs, which in a sense generalize the above.

Lastly, we draw from the 4-base variant. Take the 96 distinct vectors obtained from

$$[i\sqrt{3}\ (-1)^{j_1}\ (-1)^{j_2}\ (-1)^{j_3}\ (-1)^{j_4}\ (-1)^{-j_1-j_2-j_3-j_4}]^\top,\ \text{with } j_1,\ldots,j_4 \in [2],$$

by permuting its entries and append with the 30 obtained as the pairwise linearly independent permutations of

$$[2\ \pm 2\ 0\ 0\ 0\ 0]^\top.$$

Then the pairwise inner products have absolute value 0 or 4, and the usual construction applies.

It turns out that each of these constructions yields a gain graph that belongs to the same switching equivalence class. Will will not offer formal argumentation, but it is easily verified by computer. Note, moreover, that this is quite unsurprising, since the lines were drawn from various descriptions of the same group. Additionally, it turns out that each of the obtained gain graphs once again has all of its nonzero entries in $\mathbb{T}_6$, thus admitting a signed digraph interpretation.

7.6 Two-eigenvalue gain graphs with small degree

Having classified all two-eigenvalue gain graphs with bounded multiplicity, a relatively small collection of admissible graphs was obtained. We will now take a different perspective in bounding the degree of a candidate gain graph to a small number; this will warrant a combinatorial approach in which we will systematically investigate the potential underlying graphs and the corresponding gain functions that may act on their edges. Interestingly, for all degrees $k \leq 4$, we obtain implicit bounds on the order of our candidates.

We should note that this classification in the context of Hermitian adjacency matrices and Eisenstein matrices has essentially already been done by Greaves [45]. Foregoing the complete graphs, his constructions all have $a = 0$. However, as might be expected by now, we cannot generally make this assumption for gain graphs. Indeed, Section 7.4 contains many examples to the contrary, such as $K_{2,2,2}^{(\gamma)}$, which was obtained from 3 mutually unbiased bases in $\mathbb{C}^2$ and has distinct eigenvalues $2\sqrt{2}$ and $-\sqrt{2}$.

The results of the classification are summarized by the following theorem.

Theorem 7.24. *All two-eigenvalue gain graphs with degree at most* 4 *are switching isomorphic to one of the gain graphs in Table 7.3.*

k	Graph	Order	m	DS
2	K_3	3	1	*
	$IG(W_2)$	4	2	*
3	K_4	4	1	*
	W_4	4	2	*
	$IG(W_3)$	6	3	*
	$ND(IG(W_2))$	8	4	*
4	K_5	5	1	*
	$K_{2,2,2}^{(\gamma)}$	6	2	*
	$ND(W_4)$	8	4	*
	$IG(W_5)$	10	5	*
	$ND(IG(W_3))$	12	6	*
	$IG(W_7)$	14	7	*
	$ND(ND(IG(W_2)))$	16	8	*
	$T_{2t}^{(x)}$	$2t,\ t \geq 4$	t	

Table 7.3 – Classification of all two-eigenvalue gain graphs with degree at most 4. A star in the DS column indicates that any connected, cospectral gain graph is switching isomorphic.

In Sections 7.6.1-7.6.3, we will provide the corresponding classification for degrees

$2, 3$, and 4, respectively. Together, these sections prove the correctness of Theorem 7.24. A particularly useful insight that will be helpful in the argumentation below, is the following.

Lemma 7.25. *Let D be a connected two-eigenvalue gain graph. Then any two vertices at mutual distance* 2 *have at least two common neighbors.*

Proof. If there would be exactly one common neighbor w between non-adjacent vertices u and v, then $(A^2)_{uv} = A_{uw}A_{wv} \neq 0$. This contradicts the equation $A^2 = aA + kI$. □

Additionally, by the following observation, we may substantially limit the number of possible parameter choices in case Ψ is triangle-free.

Lemma 7.26. *Let Ψ be a connected two-eigenvalue gain graph. If Ψ is triangle-free, then $a = 0$ and thus $\theta_1 = -\theta_2$.*

Proof. $a \neq 0$ implies that $(A^2)_{uv} \neq 0$ for connected vertices u, v, and thus there is a walk $u \to w \to v$. But then $\Psi[\{u, w, v\}]$ is a triangle. □

Before we get into the actual classification, we would like to recall that it is assumed throughout that $a = \theta_1 - \theta_2 \geq 0$; that is, the eigenvalue whose multiplicity is lower is assumed to be positive. While this is a restrictive assumption, each of the graphs that are subsequently excluded may be obtained by multiplying one of the obtained graphs by -1. Hence, nothing is effectively lost.

7.6.1 Degree 2

The first relevant case to consider is, of course, $k = 2$. Without much effort, we show that there are exactly two switching equivalence classes that admit the imposed requirements.

Proposition 7.27. *Let D be a connected unit gain graph with degree $k = 2$ that has two distinct eigenvalues. Then D is switching isomorphic to K_3 or $\mathrm{IG}(W_2)$.*

Proof. Suppose that D is not a balanced triangle. Then both eigenvalues of D have multiplicity at least 2, and thus $n \geq 4$. Now, since $k = 2$, then by Lemma 7.25 we have $\Gamma(D) \cong C_4$. By Proposition 4.4, 3 out of 4 edges may be assumed to have gain one. Finally, by Lemma 7.26, $a = 0$ and thus A must satisfy the equation $A^2 = 2I$; the desired conclusion easily follows. □

7.6.2 Degree 3

Increasing the degree of the considered candidates to 3 gives us some more freedom, though the collection of switching equivalence classes is still limited to 4. The desired classification is obtained with relative ease, by application of the process described above. As was announced earlier, we find that the examples in Proposition 7.5 form a complete list.

Proposition 7.28. *Let Ψ be a connected unit gain graph with degree $k = 3$ that has two distinct eigenvalues. Then D is switching isomorphic to K_4 or one of the graphs W_4, $\mathrm{IG}(W_3)$, or the signed 3-cube $\mathrm{ND}(\mathrm{IG}(W_2))$.*

Proof. Suppose that Ψ is not switching equivalent to K_4 and let $A := A(\Psi)$. We distinguish two cases: either Ψ contains a triangle, or it does not.

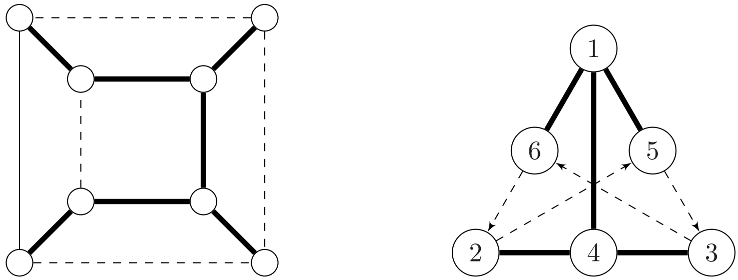
Suppose that Ψ contains a triangle. Then without loss of generality, we may assume that $A_{12} = A_{13} = A_{14} = 1$ and $A_{23} \neq 0$. Then, equating the first column of A^2 to the corresponding entries of $aA + kI$, we find that all of

$$A_{23} + A_{24} = a, \ \overline{A_{23}} + A_{34} = a, \ \text{ and } \overline{A_{24}} + \overline{A_{34}} = a$$

must simultaneously hold. Now, since a is real, it follows that $A_{23} = \overline{A_{24}} = A_{34}$ and thus that $\Gamma(\Psi) = K_4$. Indeed, since Ψ is connected and the first four vertices all have degree 3, no further vertices can be added. Moreover, since Ψ is not switching isomorphic to K_4, its eigenvalues must be $\pm\sqrt{3}$ and thus $a = 0$. Finally, using the equations above, this implies $A_{23} = \pm i$; both choices yield W_4.

If Ψ does not contain triangles, then by Lemma 7.26, $a = 0$. Moreover, by Lemma 7.25, every two vertices at distance 2 have at least two common neighbors. There are now two subcases to distinguish, and each leads to one graph. First, suppose that all pairs of vertices at distance 2 have precisely two common neighbors. Then $\Gamma(\Psi)$ is the cube [10], of which the edges marked fat in Figure 7.4a may be fixed to gain 1. Now, note that every two non-adjacent vertices of every face are connected with exactly two walks of length 2. Since the off-diagonal entries of A^2, which must be zero, are given by the sum of the gains of such a pair of walks, the gains of the non-fixed edges are all determined by the equation $A^2 = 3I$. The resulting signed graph corresponds to $\mathrm{ND}(\mathrm{IG}(W_2))$, the signed cube.

In the other case, there must be two non-adjacent vertices, say 1 and 2, that share all three neighbors. It follows that $\Gamma(\Psi) \cong K_{3,3}$; label such that $1, 2, 3$ are pairwise



(a) ND(IG(W_2)) **(b)** $IG(W_3)$

Figure 7.4 – Illustrations for Proposition 7.28. A dashed edge has gain -1; a dashed arc has gain φ.

nonadjacent. Without loss of generality, we set $A_{14} = A_{15} = A_{16} = A_{42} = A_{43} = 1$. Then, since we have

$$(A^2)_{12} = \phi(1 \to 4 \to 2) + \phi(1 \to 5 \to 2) + \phi(1 \to 6 \to 2) = 1 + A_{52} + A_{62} = 0,$$

it follows that $A_{52} = \overline{A_{62}}$ and either $A_{52} = \varphi$ or $A_{52} = \overline{\varphi}$. Moreover, since the same argument holds when $(A^2)_{13}$ is considered, we also have $A_{53} = \overline{A_{63}}$ and either $A_{53} = \varphi$ or $A_{53} = \overline{\varphi}$. Finally, since $(A^2)_{23} = 0$, we obtain $A_{52} = \overline{A_{53}}$, and thus Ψ must be precisely IG(W_3), up to equivalence. □

7.6.3 Degree 4

Proceeding along the same line, we may consider unit gain graphs with degree four. In order to gain some insight into the underlying graph, we use the following consequence of Lemma 7.1.

Lemma 7.29. *Let k be such that $1+4k$ is not a square, and let Ψ be a two-eigenvalue gain graph with degree k. Then in the underlying graph, no edge can be in exactly one triangle.*

Proof. Assume to the contrary that u and v are adjacent with precisely one common neighbor w. Without loss of generality, we may assume that $A_{uv} = A_{uw} = 1$. Then $A_{vw} = (A^2)_{uv} = a$, which is real, since $a = \theta_1 + \theta_2$, and unit, since $a = A_{vw}$. Therefore, $a = \pm 1$. But then $a \in \mathbb{N}_0$, so $a^2 + 4k$ is a perfect square, by Lemma 7.1, which is a contradiction. □

In the following classification, we first treat the case in which triangles are allowed.

Proposition 7.30. *Let D be a two-eigenvalue gain graph with degree 4. If D has triangles, then D is switching isomorphic to K_5, $\mathrm{ND}(W_4)$, $K_{2,2,2}^{(\gamma)}$, or $T_6^{(x)}$ for some unit x.*

Proof. Again, the K_5 case is clear, so let us assume that D is not switching isomorphic to a complete graph. Then both eigenvalue multiplicities are larger than 1, which implies that $n \geq 6$, since $n = 5$ would violate the absolute bound for equiangular lines in $\mathbb{C}^2$. (See Section 7.4.3.)

Since there is a triangle, we obtain by Lemma 7.29 that there must be an edge which is in precisely two triangles. Indeed, if every edge would be in 0 or more than 2 triangles, then the graph would be K_5. Without loss of generality, we may now assume that $A_{12} = A_{13} = A_{14} = A_{15} = 1$, $A_{23} = 0$, $A_{24} = x \in \mathbb{T}$, and $A_{25} \neq 0$. Now since $A_{24} + A_{25} = (A^2)_{21} = a$, for some real a, $A_{25} = a - x$. We now distinguish two cases depending on whether $a = 0$ or not, in which case $a > 0$.

For the first case, assume that $a = 0$ and thus $A_{25} = -x$. Let $y, z \in \mathbb{T} \cup \{0\}$, and without loss of generality set $A_{35} = y$, $A_{45} = z$. Since $(A^2)_{31} = 0$, it follows that $A_{34} = -y$. Moreover, since $(A^2)_{41} = 0$ and $(A^2)_{51} = 0$, it follows that

$$\overline{x} - \overline{y} + z = 0 \text{ and } -\overline{x} + \overline{y} + \overline{z} = 0, \tag{7.18}$$

and hence $z + \overline{z} = 0$. This holds true in two subcases: either $z = 0$ or $z = \pm i$.

In the former subcase, $z = 0$ and thus $x = y$. Since we may, w.l.o.g., set $A_{26} = 1$, we have

$$\begin{cases} (A^2)_{32} = A_{36} - 1 = 0 \\ (A^2)_{42} = A_{46} + 1 = 0 \\ (A^2)_{52} = A_{56} + 1 = 0 \end{cases} \implies A_{36} = -A_{46} = -A_{56} = 1,$$

and we obtain the toral tesselation graph $T_6^{(x)}$, illustrated in Figure 7.5a, with no further restrictions on x.

In the latter subcase, w.l.o.g. choose $z = i$. Applying the same technique again, we find

$$0 = (A^2)_{45} = 1 - x\overline{x} - y\overline{y} = -y\overline{y} \implies y = 0,$$

which means that $n \geq 8$, since vertex 3 needs three more neighbors. Moreover, by plugging in y and z into (7.18), it follows that $x = i$. Without loss of generality we may then assume that $A_{26} = 1$ and observe that $(A^2)_{2j} = 0$ for all j, to determine A_{j6} for $j = 3, 4, 5$. Similarly by assuming (w.l.o.g.) $A_{47} = 1$ we may determine A_{j7} for $j = 3, 5, 6$, and finally assuming $A_{58} = 1$ determines A_{j8} for $j = 3, 6, 7$. Altogether, we find a unique graph (up to switching equivalence), which was before obtained as $\mathrm{ND}(W_4)$, and is illustrated in Figure 7.5c.

In case $a > 0$, we find one more switching equivalence class through a series of similar arguments. Recall that $A_{24} = x$ and $A_{25} = a - x$. Since $a - x \in \mathbb{T}$, it follows that $a - x = \overline{x}$. Similarly, since $(A^2)_{13} = A_{43} + A_{53} = a = x + \overline{x}$, it follows that $A_{43} \in \{x, \overline{x}\}$ and $A_{53} = \overline{A_{43}}$. However, setting $A_{26} \neq 0$ w.l.o.g. and choosing $A_{43} = \overline{x}$ yields

$$(A^2)_{23} = A_{21}A_{13} + A_{24}A_{43} + A_{25}A_{53} + A_{26}A_{63} = 3 + A_{26}A_{63} \neq 0 = a \cdot A_{23},$$

where the inequality holds since $|A_{26}A_{63}| \leq 1$. Clearly, this is a contradiction and thus $A_{43} = A_{35} = x$. From $(A^2)_{14}$ it then follows similarly that $A_{45} = 0$.

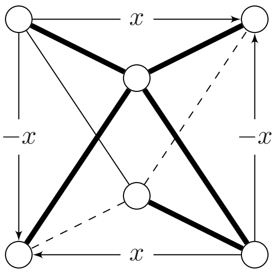
As before, we may now assume without loss of generality that $A_{26} = 1$, and determine the values A_{63}, A_{64} and A_{65} by repeating the same argument three times, as follows.

$$\begin{aligned}
1 + A_{64} = (A^2)_{24} = a \cdot A_{24} = (x + \overline{x})x = 1 + x^2 &\implies A_{64} = x^2, \\
1 + A_{65} = (A^2)_{25} = a \cdot A_{25} = (x + \overline{x})\overline{x} = 1 + \overline{x}^2 &\implies A_{65} = \overline{x}^2, \text{ and} \\
1 + \overline{x}^2 A_{63} = (A^2)_{43} = a \cdot A_{43} = (x + \overline{x})x = 1 + x^2 &\implies A_{63} = x^4.
\end{aligned}$$

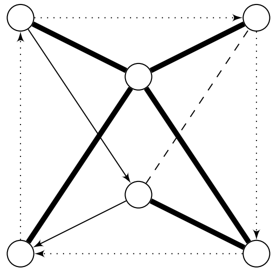
Finally, note that $(A^2)_{61} = 1 + x^2 + \overline{x}^2 + x^4 = (1 + \overline{x}^2)(1 + x^4) = 0$, which holds subject to $a = x + \overline{x} > 0$ precisely when either $x = \gamma$ or $x = \overline{\gamma}$; both cases yield $K_{2,2,2}^{(\gamma)}$, illustrated above. $\square$

The attentive reader may have noted that we did not fix the order of the above considered graphs, during the proof. However, by allowing the initially undetermined edge gains to be either complex units or zero, and following the implications, we arrive at a 4-regular gain graph in each of the possible cases. Hence, we may be certain that no larger connected examples exist.

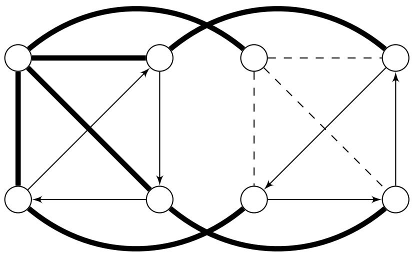
What is left is the triangle-free case. While the following result may be shown through procedure similar to the above, we opt to defer to a classification of weighing matrices by Best et al. [8], since these effectively coincide.



(a) $T_6^{(x)}$



(b) $K_{2,2,2}^{(\gamma)}$



(c) $ND(W_4)$

Figure 7.5 – Illustrations for Proposition 7.30. Filled arcs have gain i. Further edges without labels follow the usual drawing conventions.

Proposition 7.31. *Let D be a two-eigenvalue gain graph with degree 4. If D is triangle-free, then D is switching isomorphic to one of the graphs* $\mathrm{IG}(W_5)$, $\mathrm{ND}(\mathrm{IG}(W_3))$, $\mathrm{IG}(W_7)$, $\mathrm{ND}(\mathrm{ND}(\mathrm{IG}(W_2)))$, *or* $T_{2t}^{(x)}$, *for some $t > 3$ and $x \in \mathbb{T}$.*

Proof. If D is triangle-free, then by Lemma 7.26, $A := A(D)$ satisfies $A^2 = 4I$, which means that A is a weighing matrix. Thus, the results in [8, Sec. 3.5] apply, and the conclusion follows. □

It should be clear that the correctness of Theorem 7.24 now follows by Propositions 7.27, 7.28, 7.30 and 7.31. As before, the approach presented above could be expanded to include degrees $5, 6, \ldots$ with relative ease, but the abundance of possibilities would yield a discussion that is likely too lengthy to be included here.

7.6.4 Degree 5

While we will not offer a full classification, we will consider some degree-5 examples. We briefly touch on graphs of order at most 8, after which we will treat a new infinite family of two-eigenvalue gain graphs, whose underlying structure is somewhat of a doubled cycle. The remaining sporadic examples that have been found through computer search appear in Appendix 5.4.3, and will not be discussed explicitly.

Since there are exactly four 5-regular graphs of order at most 8, we may simply treat them on a case-by-case basis. For two of those candidates, namely the complement of C_8, the complement of $C_3 \cup C_5$, one may show that neither may be underlying to a two-eigenvalue gain graph. The proof follows the same pattern as the proofs of Propositions 7.30 and 7.31, so we forego the details.

The two remaining candidates, K_6 and the complement of $2C_4$, are contained in the class of donut graphs, which admit infinitely many two-eigenvalue gain graphs for every (even) order n. Let us provide the formal definition.

Definition 7.1. *Let C_t be the cycle graph of order $t \geq 3$, whose adjacency matrix is B. Then the 5-regular graph characterized by*

$$A = \begin{bmatrix} B & B+I \\ B+I & B \end{bmatrix}$$

is called the order-2t donut graph.

We will now characterize all two-eigenvalue donut graphs with symmetric spectra.

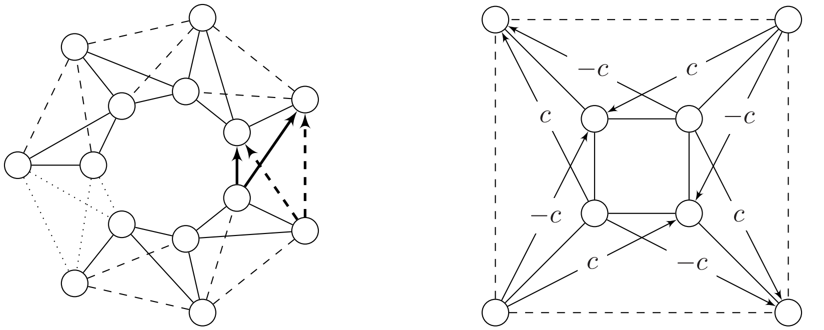
Theorem 7.32. *Let G be an order $n := 2t$ donut graph, $t \geq 3$, and let $\Psi = (G, \psi)$ be a unit gain graph. Then Ψ has eigenvalues $\pm\sqrt{5}$ if and only if it is switching isomorphic to*

$$\begin{bmatrix} C + C^* & C - C^* + I \\ C^* - C + I & -C - C^* \end{bmatrix},$$

where C is an order-t weighing matrix of weight 1, or to $D_8^*(c)$ in Figure 7.6b.

Proof. Sufficiency is clear, following the discussion in Section 7.3, so we only show necessity. If $t = 3$ then the claim holds by Theorem 7.16, so suppose that $t \geq 4$. Let C be the $t \times t$ matrix whose nonzero entries are $C_{jh} = 1$ for all $h = j + 1$ and $C_{t1} = x$ for some $x \in \mathbb{T}$. Let W, Y and Z be matrices with the same support as C, and set

$$A = \begin{bmatrix} C + C^* & W - Z^* + I \\ W^* - Z + I & Y + Y^* \end{bmatrix}.$$



(a) A general two-eigenvalue donut **(b)** $D_8^*(c)$

Figure 7.6 – Illustrations for Theorem 7.32. The fat arcs have gain $\pm x$, and dotted lines indicate continuation of the pattern.

Note that without loss of generality, $A(\Psi) = A$. Computing the upper left block of $A^2(\Psi)$ yields:

$$\begin{aligned} A^2 = 5I \quad &\Longrightarrow \quad C^2 - WZ + (C^*)^2 - Z^*W^* + W - Z + W^* - Z^* = O \\ &\Longrightarrow \quad W = Z \text{ and } C^2 + (C^*)^2 = W^2 + (W^*)^2, \end{aligned}$$

where the final equivalence follows by grouping the terms by support. Similarly, plugging in the above and computing the upper right block yields

$$\begin{aligned} A^2 = 5I \quad &\Longrightarrow \quad C + Y + C^* + Y^* + CW + WY - C^*W^* - W^*Y^* = O \\ &\Longrightarrow \quad Y = -C \text{ and } CW + W^*C^* = WC + C^*W^*. \end{aligned}$$

Now, if $t \geq 5$ then we may again group by support to reduce the final equality above to $CW = WC$. It follows that either $W = C$ or $W = -C$, completing the gain graph. Note that either choice yields the same switching equivalence class.

In case $t = 4$, all of the second order matrices have the same supports, so the above is not the only solution. Briefly put, by solving the system

$$\begin{cases} C^2 + (C^*)^2 = W^2 + (W^*)^2 \\ CW + W^*C^* = WC + C^*W^* \end{cases} \quad \Longleftrightarrow \quad \begin{cases} \overline{x} + 1 = w_{12}w_{23} + \overline{w_{34}w_{41}} \\ \overline{x} + 1 = w_{23}w_{34} + \overline{w_{12}w_{41}} \\ w_{23} + \overline{w_{41}} = w_{12} + \overline{w_{34}x} \\ w_{34} + \overline{w_{12}x} = w_{23} + \overline{w_{41}} \end{cases}$$

we obtain three options:

i. $x \in \mathbb{T}$ and $W = \pm C$,

ii. $x = -1$ and $W = \operatorname{diag}\left(\begin{bmatrix} c & \bar{c} & \bar{c} & c \end{bmatrix}\right) C$, $c \in \mathbb{T}$,

iii. $x = 1$ and $W = \operatorname{diag}\left(\begin{bmatrix} c & \bar{c} & c & \bar{c} \end{bmatrix}\right) C$, $c \in \mathbb{T}$.

The latter two yield gain graphs switching isomorphic to the exception D_8^*, shown in Figure 7.6b, which completes the proof. □

Note that indeed, K_6 is a donut, strictly speaking; though it is somewhat of a special case. In particular, since $t = 3$ implies that C^2 and C^* have the same support, the particulars of the proof above do not apply. However, as a consequence of Theorem 7.16, we know that the statement holds regardless.

Finally, note that the case $D_8^*(c)$ is distinct from the two-eigenvalue order-8 donut that follows the general construction. Indeed, the triangles in the former have gains $\pm c$, whereas the latter has triangles with gains ± 1 for all $x \in \mathbb{T}$.

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While eigenvalues of graphs are well studied, spectral analysis of complex unit gain graphs is still in its infancy. This thesis considers gain graphs whose gain groups are gradually less and less restricted, with the ultimate goal of classifying gain graphs that are characterized by their spectra. In such cases, the eigenvalues of a gain graph contain sufficient structural information that it might be uniquely (up to certain equivalence relations) constructed when only given its spectrum.

First, the first infinite family of directed graphs that is – up to isomorphism – determined by its Hermitian spectrum is obtained. Since the entries of the Hermitian adjacency matrix are complex units, these objects may be thought of as gain graphs with a restricted gain group. It is shown that directed graphs with the desired property are extremely rare. Thereafter, the perspective is generalized to include signs on the edges. By encoding the various edge-vertex incidence relations with sixth roots of unity, the above perspective can again be taken. With an interesting mix of algebraic and combinatorial techniques, all signed directed graphs with degree at most 4 or least multiplicity at most 3 are determined. Subsequently, these characterizations are used to obtain signed directed graphs that are determined by their spectra. Finally, an extensive discussion of complex unit gain graphs in their most general form is offered. After exploring their various notions of symmetry and many interesting ties to complex geometries, gain graphs with exactly two distinct eigenvalues are classified.

Pepijn Wissing (Essen, Germany, 1994) received his Bachelor's degree in Econometrics and Operations Research at Tilburg University in 2015, followed by a Research Master degree in Operations Research in 2018. He then became a PhD candidate at the department of Econometrics and Operations Research, funded in part by Tilburg University's Research Talent grant.

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