Hermitian Spectral Theory of Mixed Graphs

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Abstract

We survey existing results on Hermitian Adjacency, Hermitian Laplacian and normalised Hermitian Laplacian of mixed graphs simultaneously. We also show how to easily construct non-isomorphic mixed graphs which are cospectral with respect to all three Hermitian matrix representations.

Acknowledgements

I would like to thank my Honours Project supervisor, Dr He Sun, for introducing me to this interesting topic as well as providing constant support and expertise throughout this project.

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Chapter 1

Introduction

Spectral graph theory investigates the relationship between the structure of graphs and the eigenvalue of matrices associated, notably adjacency matrix, Laplacian matrix and normalised Laplacian matrix. In the *undirected* graphs settings, there has been extensive studies about the interplay of eigenvalues of these matrices and various graph properties, such as the diameter [Chu89, Moh91], the chromatic number [Wil67, Hof70, Cve72, Hae95], the independence number [Wil86, LZ14], bipartiteness and connectivity. Many surveys and textbooks have been written to keep track of this development [Big74, Moh91, Moh92, Mer94, Chu97, GR00, CRS09, Zha11, BH12, Bap14, Nic18]. Beyond mathematical interest, tools and techniques from spectral graph theory have provided us with many applications across computer science. This includes algorithm design and combinatorial optimization [MP93, ARV08, BSST13, Pen13, Spi17], complex network [CL06, Gag11, VM11], computer vision [SM00, Rob03], machine learning and data mining [BN03, Lux07, Sch07, Saw08, NdC11], to name a few. See also [Dra11, ACSŠ12].

In contrast, there has been relatively little result in the spectral theory of *mixed* graphs. The main reason for this is because the adjacency matrix of a mixed graph is not symmetric, unlike the case for undirected graphs. Consequently, some eigenvalues may be complex numbers, which cannot be ordered meaningfully. On the other hand, many well-known results in the undirected settings rely on studying the smallest, second smallest, second largest or largest eigenvalue of various associated matrices [CR90, CS95, Abr07, ST07, Tre12, KLL$^+$17].

In order to circumvent this, Li and Liu [LL15], and independently Guo and Mohar [GM17], introduced a different matrix representation, known as Hermitian adjacency matrix to encode the adjacency of the mixed graph. This matrix is Hermitian, and hence diagonalizable with real eigenvalues. Several interesting results on the interplay between the these eigenvalues and mixed graph structure have been given in these papers. In fact, certain results generalise from the undirected settings to the mixed graphs settings immediately by using the same proof technique. This can be seen from the statement as well as the proof method of [GM17, Proposition 4.4] in generalising Cvetković inertia bound [Cve71] (see also [GR00, Lemma 9.6.3]). On the flip side, [GM17, Corollary 7.3] shows that the diameter of a mixed graph cannot be bounded in terms of the number of distinct eigenvalues, unlike the well-behaved undirected case [BH12, Proposition 1.3.3]. Building on top of the Hermitian adjacency matrix, Hermitian Laplacian matrix and normalised Hermitian Laplacian matrix were introduced by [QY15] and [Hu18] respectively, with definitions analogous to their undirected counterparts. Beyond theoretical interest, these matrix representations of mixed graphs have recently found applications in computer science [LSZ18, MBAB18].

1.1 Objective

Although Hermitian Laplacian matrix and normalised Hermitian Laplacian matrix of mixed graphs have been introduced, results about them are relatively sparse as compared to Hermitian adjacency matrix of mixed graphs. Furthermore, the relationship between the eigenvalues of different matrices are not explicitly stated in any of the exisiting literature.

The main objective of this report is to survey existing basic results for all three matrix representations of mixed graphs simultaneously. The author believes that this integral approach makes their relationship more apparent to be appreciated. For some of the results being surveyed, the report will also comment on whether there is an analogue in the undirected setting, as well as the similarity in the proof technique used.

1.2 Main Contributions

The main contributions of the report to the existing literature are as follows:

- We found and fixed errors in Theorems 12(a) and 12(b) of [QY15]. See the discussion before Propositions 3.3.5 and 3.4.6.
- We show how to easily construct non-isomorphic mixed graphs which are cospectral with respect to all three Hermitian matrix representations. See Chapter 4.1.
- We proved an analogue of Expander Mixing Lemma for directed graphs. See Theorem 5.3.1 and Theorem 5.3.2.

1.3 Organisation

This report is organised as follows. Chapter 2 sets out the basic notations and terminology which will be used throughout the report. Chapter 3 introduces various Hermitian matrix representations of mixed graphs as well as basic results on the relationship of their eigenvalues with the graph structure. In Chapter 4, we study cospectrality of mixed graphs. In particular, we study certain kinds of graph "switching" operations which allow us to construct many non-isomorphic mixed graphs which have the same adjacency, Laplacian and normalised Laplacian spectrum. In Chapter 5, we focus on directed graphs. In particular, we look at the implications of having a low/high spectral radius on the graph structure. Chapter 6 reviews what have been done in the report as well as providing direction for future work.

Chapter 2

Preliminaries

This report assumes a good background in graph theory and linear algebra. Recommnended texts for these are [Die17] and [HJ13] respectively. When potentially advanced concept is used, we will provide pointers to other source for more information. Below we set out graph-theoretic notations and terminology which will be used throughout the report.

Let $G = (V, E)$ be a mixed graph with $V = \{v_1, v_2, \ldots, v_n\}$ and an edge set $E \subseteq V \times V$. We follow the convention that $|V| = n$ and $|E| = m$ throughout this report. Unless stated otherwise, V is always finite and there is no loops nor multiple edges in G.

We distinguish **undirected edges** as unordered pairs $\{v_j, v_k\}$ of vertices; and the **directed edges** as ordered pairs (v_j, v_k) of vertices. For any pair of vertices v_j and v_k, we write $v_j \leftrightarrow v_k$ if there is an undirected edge between them; and $v_j \to v_k$ if there is a directed edge from v_j to v_k. If all edges of a mixed graph G is undirected, we call G an **undirected graph**. Meanwhile, if all edges of a mixed graph G is directed, we call G is a **directed graph**.

The **underlying graph** of a mixed graph G, denoted by Γ_G, is the undirected graph with the same vertex set with the edge set being undirected edges that ignore the orientations in $E(G)$. Formallly, $V(\Gamma_G) = V(G)$ and $E(\Gamma_G) = \{\{v_j, v_k\} \mid \{v_j, v_k\} \in E(G)$ or $(v_j, v_k) \in E(G)\}$. The set of all mixed graphs whose underlying graph is undirected graph Γ is denoted by $\mathcal{D}(\Gamma)$. The elements of $\mathcal{D}(\Gamma)$ will be referred to as **mixed graphs based on** Γ. For a vertex $v_j \in V(G)$, the **degree** of vertex v_j, denoted by $d(v_j)$, is defined as the cardinality of the set $\{v_k \in V(G) \mid \{v_j, v_k\} \in E(\Gamma_G)\}$.

$G = K_3'$ $\qquad\qquad$ $\Gamma_G = K_3$

Figure 2.1: Mixed graph G with its underlying graph. Each vertex of G has degree 3.

Chapter 3

Hermitian Spectral Graph Theory

3.1 Hermitian Adjacency Matrix

We study the spectral theory of mixed graphs based on their Hermitian Adjacency matrix representations, which is defined as follows: Let G be a mixed graph, then the **Hermitian adjacency matrix** of G is the matrix $A = A(G) \in \mathbb{C}^{n \times n}$, where

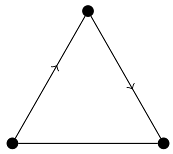
$$A_{jk} = \begin{cases} 1 & \text{if } v_j \leftrightarrow v_k; \\ i = \sqrt{-1} & \text{if } v_j \rightarrow v_k; \\ -i & \text{if } v_k \rightarrow v_j; \\ 0 & \text{otherwise.} \end{cases}$$

Notice that $A_{j,k} = \overline{A_{k,j}}$ for $1 \leq j,k \leq n$. Hence the defined adjacency matrix is Hermitian, i.e. A is equal to its conjugate transpose, A^*. This implies that A is unitarily diagonalizable with real eigenvalues. Furthermore, spectral theorem states that there exists an orthonormal basis of $\mathbb{C}^n$ that consists of eigenvectors of A. For any mixed graph G, we denote the eigenvalues of A with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. For convenience, we call this multiset the **adjacency spectrum** of G or eigenvalues of G. We further call the spectral radius of $A(G)$, i.e. $\max(|\lambda_1|, |\lambda_n|)$, as the **spectral radius** of G and denote it by $\rho(G)$. We remark that for an undirected graph Γ (as a special case of mixed graph), $A(\Gamma)$ is essentially the adjacency matrix of Γ. Hence, Hermitian adjacency matrix can be viewed as a generalisation of the well-studied adjacency matrix.

Example 3.1.1. Figure 3.1 shows us a mixed graph G and its Hermitian adjacency matrix. The adjacency spectrum of G is $\{-2, 1, 1\}$. The spectral radius of G is 2.

3.2 Basic Properties of Adjacency Spectrum

Consider forming a mixed graph G by taking the disjoint union of two mixed graphs G_1 and G_2. Since adjacency spectrum are invariant for any relabelling of vertices, we



$G = K_3'$

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

Figure 3.1: Example of a mixed graph with its Hermitian adjacency matrix

can let matrix $A(G)$ to be the direct sum of matrices $A(G_1)$ and $A(G_2)$ as illustrated in Figure 3.2.

Hence, the adjacency spectrum of G is simply the multiset sum of the adjacency spectra of G_1 and G_2. Inductively, we have the following proposition.

$$A(G) = \left[\begin{array}{c|c} A(G_1) & \mathbf{0} \\ \hline \mathbf{0} & A(G_2) \end{array}\right]$$

Figure 3.2: Hermitian adjacency matrix of disjoint union of two mixed graphs

Proposition 3.2.1. [LL15, Theorem 2.5] If a mixed graph G is a disjoint union of mixed graphs $G_1, G_2, \ldots, G_c$, then the adjacency spectrum of G is the multiset sum of the adjacency spectra of $G_1, G_2, \ldots, G_c$.

We now investigate the relationships between the sum of powers of eigenvalues and the number of cycle subgraphs in a mixed graph. Lemmas 3.2.2 and 3.2.4 are from Proposition 3.6 of [GM17] (see also [LL15, Theorem 3.1(1)]). Since these lemmas hold for undirected graphs (as special cases of mixed graphs), they generalise the well-studied corresponding results in the undirected settings, which can be found in many spectral graph theory monographs such as [BH12, Proposition 1.3.1] and [GR00, Corollary 8.1.3]. In fact, the proof technique used in the mixed graphs settings is similar to the undirected settings.

Lemma 3.2.2. [GM17, Proposition 3.6] Let G be a mixed graph and let $\lambda_1, \ldots, \lambda_n$ be its eigenvalues. Then it holds that

(i) $\displaystyle\sum_{j=1}^{n} \lambda_j = 0;$

(ii) $\displaystyle\sum_{j=1}^{n} (\lambda_j)^2 = 2m.$

Corollary 3.2.3. A mixed graph G has all eigenvalues being 0 if and only if it is a trivial graph, i.e. has no edges. In particular, if G has at least an edge, then $\lambda_1 > 0$ and $\lambda_n < 0$.

Lemma 3.2.4. [GM17, Proposition 3.6] Let G be a mixed graph, and $\lambda_1, \ldots, \lambda_n$ be its eigenvalues. We denote x_k as the number of copies of the subgraph X_k as listed in

Figure 3.3, for any $1 \leq k \leq 4$. Then it holds that

$$\sum_{j=1}^{n} (\lambda_j)^3 = 6(x_2 + x_3 + x_4 - x_1)$$

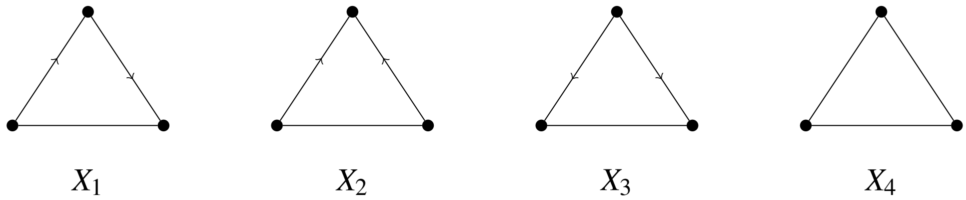


Figure 3.3: The number of subgraphs listed above, whose underlying graph is a 3-cycle, will contribute to the trace of A^3.

3.3 Spectral Radius

In this section, we study some bounds on the spectral radius of any mixed graph $G = (V, E)$. For convenience, we denote the maximum degree of a mixed graph G by $\Delta(G)$.

We first show that the spectral radius of any mixed graph G is bounded above by the biggest eigenvalue of its underlying graph in Theorem 3.3.1. Clearly, this result has no analogue in the undirected settings! That said, its proof is elementary and requires only triangle inequality.

Theorem 3.3.1. [GM17, Theorem 5.7] Let G be a mixed graph. Then $\rho(G) \leq \rho(\Gamma_G)$.

Next, we recall the well-known spectral graph theory result that the spectral radius of an undirected graph Γ is bounded above by $\Delta(\Gamma)$ in Proposition 3.3.2. The proof for the equality requires knowledge of Perron-Frobenius theorem. However, the proof for the inequality is elementary. Note that analogue of Proposition 3.3.2 doesn't hold for mixed graphs. For instance, the mixed graph K_3' in Example 3.1.1 has adjacency spectrum $\{-2, 1, 1\}$. For further discussion about mixed graphs with property $\lambda_1(G) < \rho(G)$, we refer readers to Section 5 of [GM17].

Proposition 3.3.2. [BH12, Section 3.1] For undirected graph Γ, $\rho(\Gamma) = \lambda_1(\Gamma) \leq \Delta(\Gamma)$.

By transitivity on Theorem 3.3.1 and Proposition 3.3.2, we know that the spectral radius of any mixed graph G is bounded above by $\Delta(G)$. A one-liner proof was first given for this result in [LL15, Theorem 3.1(2)] by using the rather sophisticated Gershgorin Circle Theorem. A more elementary but lengthier proof was given later in [GM17, Theorem 5.1]. And here, we presented yet another proof.

Theorem 3.3.3. For a mixed graph G, $\rho(G) \leq \Delta(G)$.

Proof. This follows immediately from Theorem 3.3.1 and Proposition 3.3.2. $\square$

We now give a lower bound for spectral radius of mixed graph.

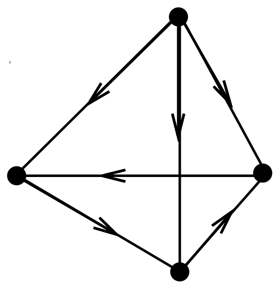
Proposition 3.3.4. Let G be a mixed graph. Let d_{avg} to be the average of the degree of all vertices in G. Then $\rho(G) \geq \sqrt{d_{avg}}$.

Proof. It follows from the handshaking lemma, Lemma 3.2.2(ii) and the definition of spectral radius that

$$\sum_{j=1}^{n} d(v_j) = 2m = \sum_{j=1}^{n} \left(\lambda_j\right)^2 \leq n(\rho(G))^2.$$

Divide both sides by n and takes the square root gives us the claim. □

Proposition 3.3.4 is tight for the directed graph K_4' in Figure 3.4. Note that this proposition implies that the well-known inequality in the undirected settings, $\rho(G) = \lambda_1 \geq d_{avg}$ [BH12, Proposition 3.12], doesn't hold in the mixed graphs settings.



$$A(K_4') = \begin{bmatrix} 0 & i & i & i \\ -i & 0 & -i & i \\ -i & i & 0 & -i \\ -i & -i & i & 0 \end{bmatrix}$$

Figure 3.4: K_4' with adjacency spectrum $\{-\sqrt{3}, -\sqrt{3}, \sqrt{3}, \sqrt{3}\}$.

We would also like to point out that K_4' in Figure 3.4 seems to contradict the claim in Theorem 12(a) of [QY15]. Theorem 12(a) of [QY15] claims that for a mixed graph G, it holds that $\sqrt{\Delta(G)+1} \leq \lambda_1$. Applying the claim to K_4', we have $2 = \sqrt{3+1} \leq \sqrt{3}$, which is absurd. Scrutinising the proof , we found a careless mistake on the line

"*By Theorem 8, we have* $\lambda_1(M) \geq \lambda_1(K_{1,\Delta}) = \sqrt{\Delta+1}$"

It is well-known that for star graph $S_n = K_{1,\Delta}$, we have $\lambda_1(K_{1,\Delta}) = \sqrt{\Delta}$ instead of $\sqrt{\Delta+1}$. Once this is fixed, the proof works fine. We remark that this proposition generalises the corresponding result in the undirected settings, using a similar proof [CR90].

Proposition 3.3.5. [QY15, Theorem 12(a)] Let G be a mixed graph with maximum degree Δ. Then $\lambda_1(G) \geq \sqrt{\Delta}$.

3.4 Hermitian and Normalised Hermitian Laplacian Matrix

In the spectral theory of undirected graphs, there are other matrix representations which are well-studied besides adjacency matrix representation. Two very common representations are known as the Laplacian matrix representations and normalised Laplacian matrix representation. The spectrum of these matrices have many useful properties and applications. For instance, the second smallest eigenvalue of both these matrices can be used to approximate the sparsest cut of a graph [AM85a, Alo86]. They have been used to construct low dimensional embeddings [NdC11], which are useful for a variety of machine learning applications. Motivated by this, we study similar matrix representations in the mixed graphs settings.

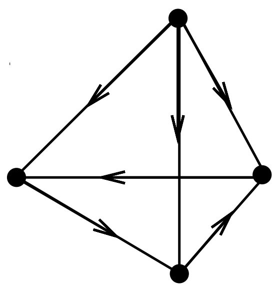
3.4.1 Hermitian Laplacian Matrix

The **Hermitian Laplacian matrix** of a mixed graph G is the matrix $L = L(G) \in \mathbb{C}^{n\times n}$ defined by $L = D - A$, where D is the diagonal matrix defined by $D_{jj} = d(v_j)$ and A is the Hermitian adjacency matrix of G. More explicitly, we have

$$L_{jk} = \begin{cases} d(v_j) & \text{if } j = k; \\ -A_{jk} & \text{otherwise.} \end{cases}$$

It is clear that any Hermitian Laplacian matrix L is Hermitian. Thus, L is also unitarily diagonalizable with real eigenvalues. For any mixed graph G, we denote the eigenvalues of L with $\tau_1 \le \tau_2 \le \cdots \le \tau_n$. We call this multiset the **Laplacian spectrum** of G. It is clear that we have an analogue of Proposition 3.2.1 for Laplacian spectrum. Note that we are following the convention of denoting the Laplacian spectrum in an increasing order.

Example 3.4.1. Reusing K_4' as example, we have its Laplacian matrix as below.



$$L(K_4') = \begin{bmatrix} 3 & -i & -i & -i \\ i & 3 & i & -i \\ i & -i & 3 & i \\ i & i & -i & 3 \end{bmatrix}$$

Figure 3.5: K_4' with Laplacian spectrum $\{3-\sqrt{3}, 3-\sqrt{3}, 3+\sqrt{3}, 3+\sqrt{3}\}$.

Proposition 3.4.2. If a mixed graph G is a union of mixed graphs $G_1, G_2, \ldots, G_c$, then the Laplacian spectrum of G is the multiset sum of the Laplacian spectra of $G_1, G_2, \ldots, G_c$.

Applying handshaking lemma on the trace of L, we immediately get the following proposition. This clearly holds in the undirected settings.

Proposition 3.4.3. Let G be a mixed graph. Then $\sum_{j=1}^{n} \tau_j = \sum_{j=1}^{n} d(v_j) = 2m$.

Furthermore, L is a positive semi-definite matrix, i.e. all its eigenvalues are non-negative. This is first proved in [QY15, Theorem 9]. A different proof is given in Remark 1 of the same paper. This theorem is a generalisation of the corresponding theorem in the undirected settings [AM85b]. That said, both proof techniques used in [QY15] are similar to the proofs used in the undirected settings (see [GR00, page 280] and [Nic18, Formula 7.2]).

Theorem 3.4.4. [QY15, Theorem 9] The Hermitian Laplacian matrix of any mixed graph is a positive semi-definite matrix.

We remark that although $\tau_1 = 0$ is *always* an eigenvalue of the Laplacian matrix in undirected settings [GR00, page 280], this is not the case for mixed graphs. We are only certain that $\tau_1 \geq 0$ for mixed graphs. For instance, K_4' in Figure 3.5 has a Laplacian spectrum of $\{3-\sqrt{3}, 3-\sqrt{3}, 3+\sqrt{3}, 3+\sqrt{3}\}$.

Proposition 3.4.3 and Theorem 3.4.4 give us some bounds on τ_2. Of course, this bound holds for undirected graphs as well using an identical proof.

Proposition 3.4.5. Let G be a mixed graph. Then $\tau_2 \leq 2m/(n-1)$.

Proof. Since $\tau_1 \geq 0$, we have $\sum_{j=2}^{n} \tau_j \leq 2m$. Hence, we have $\tau_2 \leq 2m/(n-1)$. □

We would like to point out that the claim in Theorem 12(b) of [QY15] is again, careless. Theorem 12(b) of [QY15] claims that for a mixed graph G, it holds that $\Delta(G)+1 \leq \tau_n$. There is a trivial counter example: G is a mixed graph with a vertex but no edges. It is clear that $\Delta(G) = 0 = \tau_n(G)$. This implies $1 \leq 0$, which is absurd. The statement can be fixed by adding the condition of "Let G be a mixed graph with at least one edge." Now the statement and the proof work fine. This result also generalise from the undirected settings, using a similar proof [GM94, Corollary 2].

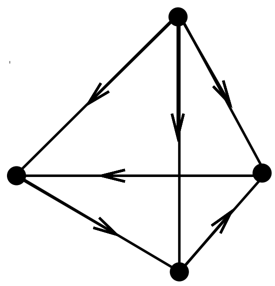
Proposition 3.4.6. [QY15, Theorem 12(b)] Let G be a mixed graph with at least one edge. Denote the maximum degree of G by Δ. Then $\Delta + 1 \leq \tau_n(G) \leq 2\Delta$.

3.4.2 Normalised Hermitian Laplacian Matrix

Let G be a mixed graph with Hermitian Laplacian matrix L. The **normalised Hermitian Laplacian matrix** of G is the matrix $\mathcal{L} = \mathcal{L}(G) \in \mathbb{C}^{n\times n}$ defined by $\mathcal{L} = D^{-1/2}LD^{-1/2}$, where $D^{-1/2}$ is the diagonal matrix defined by $\left(D^{-1/2}\right)_{jj} = \sqrt{d(v_j)}$. More explicitly, we have

$$\mathcal{L}_{jk} = \begin{cases} 1 & \text{if } j = k \text{ and } d(v_j) \neq 0; \\ -\dfrac{A_{jk}}{\sqrt{d(v_j)d(v_k)}} & \text{if } j \neq k \text{ and } v_j \text{ is adjacent to } v_k; \\ 0 & \text{otherwise.} \end{cases}$$

Example 3.4.7. Reusing K_4' as example, we have its normalised Laplacian matrix as below.



$$\mathcal{L}(K_4') = \begin{bmatrix} 1 & -i/3 & -i/3 & -i/3 \\ i/3 & 1 & i/3 & -i/3 \\ i/3 & -i/3 & 1 & i/3 \\ i/3 & i/3 & -i/3 & 1 \end{bmatrix}$$

Figure 3.6: K_4' with normalised Laplacian spectrum $\{1-\sqrt{3}/3,\ 1-\sqrt{3}/3,\ 1+\sqrt{3}/3,\ 1+\sqrt{3}/3\}$.

It is clear that any normalised Hermitian Laplacian matrix $\mathcal{L}$ is Hermitian. Thus, $\mathcal{L}$ is unitarily diagonalizable with real eigenvalues. For any mixed graph G, we denote the eigenvalues of $\mathcal{L}(G)$ with $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_n$. We call this multiset the **normalised Laplacian spectrum** of G. It is clear that we have an analogue of Proposition 3.2.1 for normalised Laplacian spectrum.

Proposition 3.4.8. If a mixed graph G is a union of mixed graphs $G_1, G_2, \ldots, G_c$, then the normalised Laplacian spectrum of G is the multiset sum of the Laplacian spectra of $G_1, G_2, \ldots, G_c$.

Observe that $\mathrm{tr}(\mathcal{L})$ is the number of non-isolated vertices, which is bounded above by n. Hence, the sum of normalised Laplacian spectrum is at most n. It is also clear that each trivial component of a mixed graph (consisting only an isolated vertex) contributes a 0 to the normalised Laplacian spectrum. Furthermore, when G has no isolated vertices, we have $\mathcal{L} = I_n - D^{-1/2}AD^{-1/2}$. In this case, $\mathrm{tr}(\mathcal{L}) = n$.

Similar to (unnormalised) Laplacian matrix, $\mathcal{L}$ is also a positive semi-definite matrix. This is first proved in [Hu18, page 113]. This theorem is also the generalisation of the theorem in the undirected setting, using a similar proof technique [Chu97, Equation 1.1]. We also remark that although 0 is *always* an eigenvalue of the normalised Laplacian matrix in undirected settings [Chu97, page 4], this is not the case for mixed graphs. For instance, K_4' in Figure 3.6 has a normalised Laplacian spectrum of $\{1-\sqrt{3}/3,\ 1-\sqrt{3}/3,\ 1+\sqrt{3}/3,\ 1+\sqrt{3}/3\}$.

Theorem 3.4.9. [Hu18, page 113] The normalised Hermitian Laplacian matrix of any mixed graph is a positive semi-definite matrix.

In fact, the normalised Laplacian spectrum is bounded above by 2. This is first proved in [Hu18, page 114]. Again, this is also the generalisation of the theorem in the undirected setting using a similar proof technique [Chu97, Lemma 1.7(v)].

Theorem 3.4.10. [Hu18, page 114] The eigenvalues of the normalised Hermitian

Laplacian matrix of any mixed graph is at most 2.

Similar to the undirected graphs settings, for mixed graph G with no isolated vertices, we can relate the adjacency spectrum and normalised Laplacian spectrum by applying Sylvesters law of inertia [Cav10, page 25]. For more details about Sylvesters law of inertia, see [HJ13, Theorem 4.5.8])

Proposition 3.4.11. Let G be a mixed graph with no isolated vertices. Then t he multiplicity of 0 as an eigenvalue for A equals the multiplicity of 1 as an eigenvalue for $\mathcal{L}$. Furthermore, the number of positive (resp. negative) eigenvalue of A corresponds to the number of eigenvalues of $\mathcal{L}$ in $[0,1)$ (resp. $(1,2]$) for $\mathcal{L}$.

Proof. The proof follows immediately from applying Sylvesters law of inertia to the matrix $I-\mathcal{L}$ and A. $\square$

Chapter 4

Cospectrality

We say two mixed graphs G_1 and G_2 are **isomorphic** if they are the "same" graph up to relabelling. Formally, G_1 and G_2 are isomorphic if there is a permutation matrix such that $A(G_1) = PA(G_2)P^{\intercal}$. It is clear that two isomorphic mixed graphs have the same Hermitian adjacency, Laplacian and normalised Laplacian spectrum. However, the converse is not true.

In spectral theory of undirected graph, it is well known that there are non-isomorphic undirected graphs which share the same adjacency spectrum. The smallest such pair of graphs have 5 vertices each, as shown in Figure 4.1 [VCS57]. Each of them has the adjacency spectrum of $\{-2, 0, 0, 0, 2\}$. Notice also that the first graph in Figure 4.1 is not connected while the second graph is connected. Therefore, we see that having the same adjacency spectrum does not translate to having the same connectivity properties.

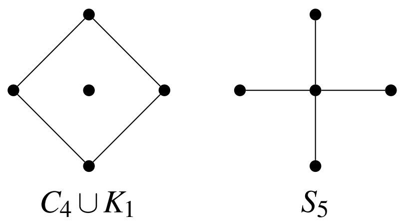


Figure 4.1: The smallest pair of non-isomorphic cospectral undirected graphs.

In this report, we say two mixed graphs are **cospectral** if they have the same *adjacency* spectrum. Clearly, any pair of cospectral but non-isomorphic undirected graph such as Figure 4.1 is a pair of cospectral non-isomorphic mixed graph. We remark that there exist mixed graphs which share the same adjacency spectrum but not Laplacian and normalised Laplacian spectrum. Figure 4.1 gives an easy example.

The smallest pair of non-isomorphic cospectral mixed graphs (4 vertices and 3 edges) with non-isomorphic *underlying graph* is as shown in Figure 4.2 below. Furthermore, we observe from Figure 4.3 that although mixed graphs G_1, G_2 and G_3 are cospectral, they are connected, weakly connected, and disconnected respectively. Therefore, we see that cospectrality doesn't translate to sharing the same connectivity properties for mixed graphs.

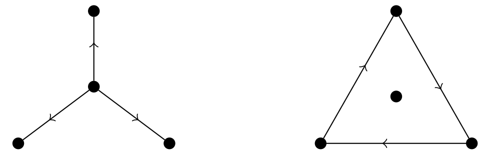


Figure 4.2: The smallest pair of cospectral mixed graph with non-isomorphic underlying graph [GM17, Figure 10].

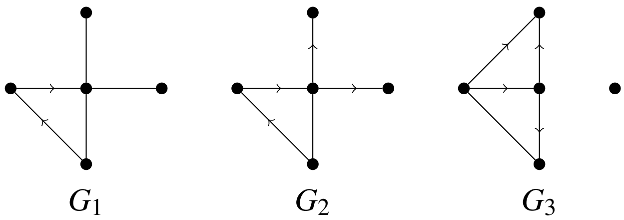


Figure 4.3: Cospectral mixed graphs with different connectivity properties [GM17, Figure 9].

Observe G_1 and G_2 in Figure 4.3 are non-isomorphic even though they are cospectral and share a same underlying graph. The smallest pair of such non-isomorphic cospectral mixed graphs is given in Figure 4.4, which both have adjacency spectrum of $\{-1,1\}$.

Figure 4.4: The smallest pair of non-isomorphic cospectral mixed graphs.

In Chapter 4.1, we will investigate in details on cospectral mixed graphs which share the same underlying graph. This involves studying various graph "switching" operation that preserve spectrum and underlying graph. Later on in Chapter 4.2, we focus on mixed graphs which are cospectral with their underlying graph.

4.1 Cospectrality within $\mathcal{D}(\Gamma)$

Consider two cospectral mixed graphs G and G' which have the same underlying graph. One way to describe G' is by describing the changes required to make on each edge in $E(G)$. For instance, we can change certain directed edge to an undirected edge, reverse the direction of an directed edge, etc.

It is natural to ask if there is a general structure behind graph operations that output a cospectral graph of the input mixed graph. In this section, we will investigate two different types of graph operations that output a cospectral graph of the input mixed graph. Interestingly, the output mixed graphs of both types have the same Laplacian and normalised Laplacian spectrum as the input mixed graph (see Propositions 4.1.2 and 4.1.4). This allows us to easily construct many non-isomorphic mixed graphs which have the same adjacency, Laplacian and normalised Laplacian spectrum.

4.1.1 Converse Graph is Cospectral

Our first type of graph operation is rather straightforward: reverse the direction of each directed edge, i.e. the output graph is the converse graph. Observe that for a mixed graph G, we have $A(G^*) = [A(G)]^\intercal$. Since a square matrix is similar to its transpose, we immediately have the following proposition.

Proposition 4.1.1. [GM17, Proposition 8.1] A mixed graph G and its converse are cospectral.

In fact, G^* shares the same Laplacian and normalised Laplacian spectrum with G as well.

Proposition 4.1.2. A mixed graph G and its converse have the same Laplacian and normalised Laplacian spectrum.

Proof. For convenience, we write $A = A(G)$ and $D = D(G) = D(G^*)$. Note that $A^\intercal = A(G^*)$ and $D^\intercal = D$. We then have

$$L(G^*) = D^\intercal - A^\intercal = (D-A)^\intercal = [L(G)]^\intercal.$$

As a square matrix is similar to its transpose, the claim follows.

Similarly, for normalised Laplacian matrix, we have

$$\begin{aligned}
\mathcal{L}(G^*) &= D^{-1/2} L(G^*) D^{-1/2} \\
&= \left(D^{-1/2}\right)^\intercal [L(G)]^\intercal \left(D^{-1/2}\right)^\intercal \\
&= \left(D^{-1/2} L(G) D^{-1/2}\right)^\intercal \\
&= \mathcal{L}(G)^\intercal
\end{aligned}$$

□

While the graph operation of taking converse can be applied to any mixed graph, it is rather limited and provides us at most one cospectral graph of G. For instance, the graph operation required to obtain K_2 from K_2' in Figure 4.4 is not included.

4.1.2 Graph Switching

In contrast to the graph operation of taking converse, our next type of cospectral graph operations is rather complicated. This idea was first shown in page 23 of [GM17]. Algebraically, the graph operations are represented by *similarity transformations* through invertible diagonal matrices. Furthermore, we will show that these graph operations preserve the Laplacian and normalised Laplacian spectrum.

We first describe the edge relations required. Let G be a mixed graph. Suppose that its vertex set V is partitioned into 4 (possibly empty) sets, V_1, V_i, V_{-1}, V_{-i}, i.e. $V = \bigcup_{r=0}^{3} V_{i^r}$.

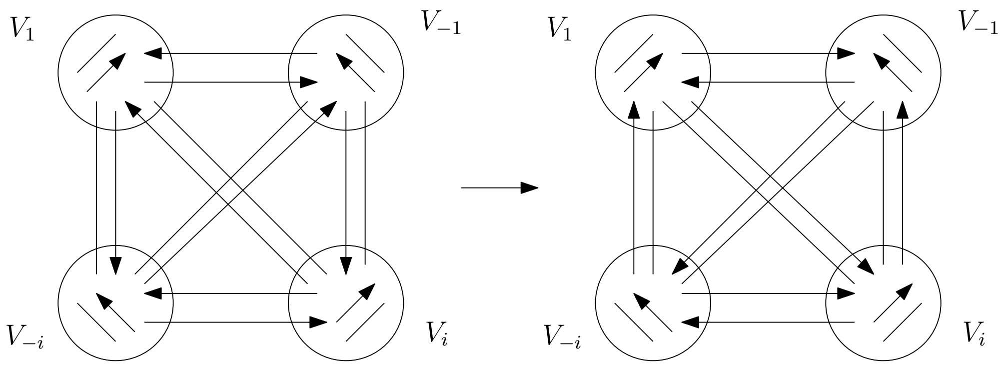


Figure 4.5: Four-way switching on the admissible edges. [GM17, Figure 11]

An undirected edge $\{v_j, v_k\}$ or a directed edge (v_j, v_k) is said to be of type (ω_1, ω_2) if $v_j \in V_{\omega_1}$ and $v_k \in V_{\omega_2}$ for $\omega_1, \omega_2 \in \{1, i, -1, -i\}$. We say a partition of vertex set V is **admissible** if all of the following conditions hold:

(i) each edge must be of type $(\omega,\omega), (\omega, i\omega), (\omega, -i\omega), (\omega, -\omega)$;

(ii) each edge of type $(\omega, i\omega)$ is an undirected edge;

(iii) each edge of type $(\omega, -i\omega)$ is a directed edge from V_ω to $V_{-i\omega}$;

(iv) each edge of type $(\omega, -\omega)$ is a directed edge from V_ω to $V_{-\omega}$.

We now describe the graph operations. Let G be a mixed graph. A **four-way switching** with respect to partition $V(G) = \bigcup_{r=0}^{3} V_{i^r}$ is a graph operation of changing G into a mixed graph G' by making the following changes:

(i) reversing the direction of each directed edge of type $(\omega, -\omega)$;

(ii) replacing each undirected edge of type $(\omega, i\omega)$ with a directed edge from V_ω to $V_{i\omega}$;

(iii) replacing each directed edge of type $(\omega, -i\omega)$ with an undirected edge of type $(-i\omega, \omega)$.

We are now ready to state [GM17, Theorem 8.5], which proves that if admissibility is satisfied, then the adjacency spectrum is preserved under four-way switching operation. We will sketch a proof below as certain notions used in the proof is required to prove Proposition 4.1.4.

Theorem 4.1.3. [GM17, Theorem 8.5] Let G be a mixed graph such that the partition of its vertex set $V = \bigcup_{r=0}^{3} V_{i^r}$ is admissible. Let G' be the mixed graph obtained from G through the four-way switching operation. Then, G and G' are cospectral.

Proof Sketch. Define a diagonal matrix $S \in \mathbb{C}^{n\times n}$ such that $S_{jj} = \omega \in \{1, i, -1, -i\}$ if $v_j \in V_\omega$. For brevity, we write $A = A(G)$ and $A' = A(G')$. Define a matrix $B = S^{-1}AS$.

Then, for an arbitrary pair of vertex v_j and vertex v_k, we can verify that

$$B_{jk} = A_{jk}\frac{S_{kk}}{S_{jj}} = \overline{B_{kj}}.$$

Thus, B is a well-defined Hermitian adjacency matrix of a mixed graph with the same underlying graph as G, which is due to the admissibility of V. We are left with verifying that the similarity transformation correctly represents the four-way switching operation, i.e. $A'_{jk} = B_{jk}$ for all j,k. $\square$

Proposition 4.1.4. Let G and G' be mixed graphs as in Theorem 4.1.3, then G has the same Laplacian and normalised Laplacian spectrum with G'.

Proof. For convenience, we write $A = A(G)$, $A' = A(G')$, $L = L(G)$, $L' = L(G')$, $\mathcal{L} = \mathcal{L}(G)$, $\mathcal{L}' = \mathcal{L}(G')$ and $D = D(G) = D(G')$. From the proof sketch of Theorem 4.1.3, we have $A' = S^{-1}AS$ for some invertibe diagonal matrix S. We have

$$\begin{aligned}
L' &= D - A' \\
&= D - S^{-1}AS \\
&= S^{-1}SD - S^{-1}AS \\
&= S^{-1}DS - S^{-1}AS \\
&= S^{-1}(D-A)S \\
&= S^{-1}LS.
\end{aligned}$$

Note that the fourth equality is due to diagonal matrices commute under matrix multiplication. As L' and L are similar matrices, G and G' have the same Laplacian spectrum.

Similar analysis on $\mathcal{L}'$ gives us

$$\begin{aligned}
\mathcal{L}' &= D^{-1/2}L'D^{-1/2} \\
&= D^{-1/2}\left(S^{-1}LS\right)D^{-1/2} \\
&= S^{-1}\left(D^{-1/2}LD^{-1/2}\right)S \\
&= S^{-1}\mathcal{L}S.
\end{aligned}$$

Thus, G and G' have the same normalised Laplacian spectrum. $\square$

Consider an undirected forest F and a mixed graph $G \in \mathcal{D}(F)$. We can change each edge in F to match the edge type in G through repeated four-way switchings. We will illustrate how to do this through an example. Suppose we want to change an edge $\{u,v\}$ of F from an undirected edge to a directed edge (u,v). Then we can partition the vertices of F into V_1 and V_i such that $u \in V_1$ and $v \in V_i$ and $\{u,v\}$ is an cut-edge. The four-way switching will change $\{u,v\}$ to (u,v) while all the other edges are unaffected. Since this partition is admissible, we have the adjacency spectrum preserved after the switching. Similar analysis applies to other types of edge change. Inductively, we can change each edge in F to become G eventually, while preserving the adjacency spectrum throughout the process.

This gives us the following corollary which was first proved in [LL15, Corollary 2.21]. The proof idea in the paragraph above is based on the proof in [GM17, Corollary 8.4].

Corollary 4.1.5. [LL15, Corollary 2.21] Let F be a forest. Then all mixed graphs whose underlying graph is F are cospectral with F.

Proposition 4.1.4 allows to strengthen the claim in Corollary 4.1.5.

Corollary 4.1.6. Let F be a forest. Then all mixed graphs whose underlying graph is F have the same Laplacian and normalised Laplacian spectrum with F.

4.1.3 Switching Equivalence

Suppose G' can be obtained from G by applying a sequence of four-way switchings and operations of taking the converse. We say these two mixed graphs are **switching equivalent**. Proposition 3.3 in [Moh16] shows that two mixed graphs G and G' being switching equivalent is in fact an equivalence relation on the set $\mathcal{D}(\Gamma_G)$.

Proposition 4.1.7. [Moh16, Proposition 3.3] Let Γ be an undirected graph. Then, switching equivalence is an equivalence relation on the set $\mathcal{D}(\Gamma)$. Furthermore, for all $G \in \mathcal{D}(\Gamma)$, switching equivalence class of G contains all mixed graphs that are obtained from G or G^* by a *single application* of four-way switching operation.

Proposition 4.1.8. If mixed graphs G and G' are switching equivalent, then G has the same Laplacian and normalised Laplacian spectrum with G'.

Proof. From Proposition 4.1.7, either G' is obtained from G or G^* by a single application of a four-way switching. For the first case, the claim follows immediately from Proposition 4.1.4.

For the second case, Proposition 4.1.1 gives us G and G^* have the same Laplacian and normalised Laplacian spectrum, while Proposition 4.1.4 gives us G^* and G' have the same Laplacian and normalised Laplacian spectrum. The claim follows. $\square$

It is clear that two switching equivalent graphs necessarily have the same underlying graph. However, we are not sure if two cospectral graph with the same underlying graph are necessarily switching equivalent. Hence, we would like to propose the following problem:

Problem 4.1.9. For any mixed graph G, are the following conditions equivalent?

(i) G' is switching equivalent to G;

(ii) $G' \in \mathcal{D}(\Gamma_G)$ and G' is cospectral to G.

4.2 Mixed Graphs Which are Cospectral to Their Underlying Graph

If a pair of mixed graphs G and G' are switching equivalent, then they share the same underlying graph, i.e. $\Gamma_G = \Gamma_{G'}$. As stated in Problem 4.1.9, we are not sure if there exist cospectral graphs G and G' such that $\Gamma_G = \Gamma_{G'}$, but G and G' are not switching equivalent. However, much more can be said if a mixed graph is cospectral to its underlying graph. In this section, we show that for any undirected graph Γ, all mixed graphs $G \in \mathcal{D}(\Gamma)$ which are cospectral to Γ are switching equivalent to each other.

We first show in Theorem 4.2.1 that for a *connected* (undirected) graph Γ, a mixed graph $G \in \mathcal{D}(\Gamma)$ is cospectral to Γ if and only if G and Γ are switching equivalent. This allows us to deduce in Corollary 4.2.2 that for a connected graph Γ, if G and $G' \in \mathcal{D}(\Gamma)$ are both cospectral to Γ, then G and G' are switching equivalent. We then generalize this to all undirected mixed graph using mathematical induction on the number of components.

The next theorem is first shown in [Moh16, Theorem 4.1].

Theorem 4.2.1. [Moh16, Theorem 4.1] Let Γ be a connected undirected graph. Let G be a mixed graph obtained from Γ by deleting some edges and orienting a subset of the remaining edges. The following statements are equivalent:

(i) G and Γ are cospectral.

(ii) $\lambda_1(G) = \lambda_1(\Gamma)$.

(iii) None of the edges have been deleted and there exists a partition of the vertex-set of G into 4 (possibly empty) parts V_1, V_i, V_{-1}, V_{-i} such that the following holds. For $\omega \in \{1, i, -1, -i\}$, the subgraph induced by V_ω in G contains only undirected edges. Every other edges of G is a directed edge from V_ω to $V_{-i\omega}$ for some $\omega \in \{1, i, -1, -i\}$. See Figure 4.6.

(iv) G and Γ are switching equivalent.

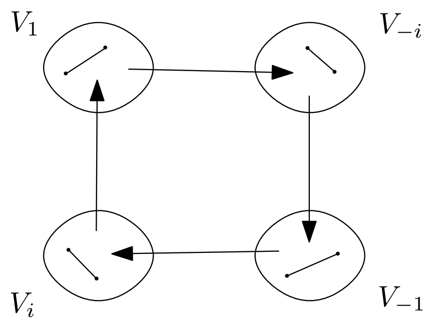


Figure 4.6: Structure from Theorems 4.2.1(iii) [Moh16, Figure 3].

It is clear from Theorem 4.2.1 that for a connected undirected graph Γ, a mixed graph $G \in \mathcal{D}(\Gamma)$ is cospectral to Γ if and only if G and Γ are switching equivalent. Since switching equivalence is an equivalence relation on the set $\mathcal{D}(\Gamma)$, we have the following corollary.

Corollary 4.2.2. Let Γ be a connected undirected graph and G, $G' \in \mathcal{D}(\Gamma)$. If G and G' are both cospectral to Γ, then G and G' are switching equivalent.

Recall that the smallest eigenvalue for Laplacian and normalised Laplacian matrix of undirected graph is always 0. Together with Proposition 4.1.8 and Theorem 4.2.1, we can deduce the following.

Corollary 4.2.3. Let Γ be a connected undirected graph. If mixed graph $G \in \mathcal{D}(\Gamma)$ is cospectral with Γ, then $\tau_1(G) = \mu_1(G) = 0$.

In fact, the converse is true as well.

Theorem 4.2.4. [QY15, Theorem 10] Let G be a connected mixed graph. If $\tau_1(G) = 0$ or $\mu_1(G) = 0$, then G is cospectral with Γ_G.

To summarise, for a weakly connected mixed graph $G = (V,E)$, the following conditions are equivalent.

(i) G is cospectral to Γ_G.

(ii) $\lambda_1(G) = \lambda_1(\Gamma_G)$.

(iii) There exists a partition of V into 4 (possibly empty) parts V_1, V_i, V_{-1}, V_{-i} such that the following holds. For $\omega \in \{1, i, -1, -i\}$, the subgraph induced by V_ω in G contains only undirected edges. Every other edges of G is a directed edge from V_ω to $V_{-i\omega}$ for some $\omega \in \{1, i, -1, -i\}$. See Figure 4.6.

(iv) G and Γ_G are switching equivalent.

(v) G has the same Laplacian spectrum as Γ_G.

(vi) G has the same normalised Laplacian spectrum as Γ_G.

(vii) $\tau_1(G) = 0$.

(viii) $\mu_1(G) = 0$.

We emphasize that Theorem 4.2.1 and Theorem 4.2.4 are true only for weakly connected mixed graph. In particular, conditions (ii), (vii) and (viii) of the summary above are necessary but not sufficient conditions for a mixed graph G to be cospectral to Γ_G.

In fact, it is easy to construct counterexample: Let G be the disjoint union of mixed graphs G_1 and G_2, where G_1 is cospectral to Γ_{G_1} but G_2 isn't cospectral to Γ_{G_2}. Applying Proposition 3.2.1 to $G = G_1 \cup G_2$ and $\Gamma_G = \Gamma_{G_1} \cup \Gamma_{G_2}$, we see that G is not cospectral to Γ_G. However, Propositions 3.4.2 and 3.4.8, together with the fact that G_1 is cospectral to Γ_{G_1} gives us $\tau_1(G) = \mu_1(G) = 0$.

Fortunately, the remaining conditions can be extended to mixed graphs which are not weakly connected, using mathematical induction and Proposition 3.2.1.

Theorem 4.2.5. Let Γ be an undirected graph with c components, i.e. Γ is a union of undirected graphs $\Gamma_1, \Gamma_2, \ldots, \Gamma_c$. Suppose a mixed graph $G \in \mathcal{D}(\Gamma)$ is cospectral to Γ. Then G is switching equivalent to Γ.

Proof. We denote G_j as the component corresponds to Γ_j for $j = 1, \ldots, c$. Since G is cospectral to Γ, we have $\lambda_1(G) = \lambda_1(\Gamma)$.

We first notice that there exists some j where $1 \leq j \leq c$, such that $\lambda_1(G_j) = \lambda_1(G) = \lambda_1(\Gamma) = \lambda_1(\Gamma_j)$. This must be true as otherwise we will have $\lambda_1(G_j) > \lambda_1(\Gamma_j)$ for some j. But then this implies $\rho(G_j) \geq \lambda_1(G_j) > \lambda_1(\Gamma_j) = \rho(\Gamma_j)$. which contradicts Theorem 3.3.1.

Applying Theorem 4.2.1 on G_j and Γ_j, we have G_j and Γ_j are switching equivalent. Thus, we can get Γ_j from G_j through four-way switching operation. We now consider the remaining graph components, i.e. the mixed graph $G - G_j$ and the undirected graph $\Gamma - \Gamma_j$. Repeating the same argument inductively, we have each component of G is switching equivalent to its corresponding component in Γ. It follows easily that we can get Γ from G through four-way switching operations and hence G is switching equivalent to Γ. □

Corollary 4.2.6. Let Γ be an undirected graph and G, $G' \in \mathcal{D}(\Gamma)$. If G and G' are both cospectral to Γ, then G and G' are switching equivalent.

Chapter 5

Structure and Randomness in Directed Graphs

In this chapter, we will focus only on directed graphs. In Section 5.1, we will look at what extra eigenvalues properties do directed graphs possess. In Section 5.2, we revisit earlier studies on cospectrality for mixed graphs by restricting them to directed graphs. In Section 5.3, we investigate the graph properties of directed graphs which possess low μ_n. In Section 5.4, we look at Quasi-randomness conditions for directed graphs from the perspective of spectral radius and netflow. In Section 5.5, we study the upper bound for the minimum spectral radius among all directed graphs with the same underlying graph.

Skew-Adjacency Matrix of Directed Graphs

Before Hermitian adjacency matrix was introduced to study mixed graphs, a matrix representation known as skew-adjacency matrix of directed graphs was introduced to study directed graphs [CCF+12]. Instead of using $\pm i$ to encode the directed edges, the skew-adjacency matrix uses ± 1. It is clear that if we use Hermitian adjacency matrix to study only directed graphs, then these two matrix representation are essentially the same up to scalar multiple of i. In particular, the spectrum are purely imaginary, which can be harmlessly made real by multiplying by $-i$. That said, skew-adjacency matrix representation has a big disadvantage: if we try to define skew Laplacian matrix "naturally" by taking off the adjacency matrix from the degree matrix, then the resulting Laplacian matrix is not necessarily diagonalisable with real eigenvalues.

5.1 Directed Graphs and their Spectrum

Let G be a directed graph with adjacency matrix A. In fact, the adjacency spectrum of a directed graph G is symmetric about 0. Two rather different proofs are given by

[LL15, Corollary 2.13] and [GM17, Theorem 6.2].

The proof given by [LL15, Corollary 2.13] is an easy corollary of [LL15, Theorem 2.8], which gives an explicit formula for the coefficients of the characteristic polynomial of A based on the combinatorial properties of G. Meanwhile, the proof given by [GM17, Theorem 6.2] requires only basic algebra. We present another proof here, which requires only elementary linear algebra.

Proposition 5.1.1. The adjacency spectrum of a directed graph G is symmetric about 0.

Proof. Notice that $A_{jk} = -A_{kj}$ for all $1 \leq j,k \leq n$. Thus, A is skew-symmetric, i.e. $A^\intercal = -A$. Since A is similar to $A^\intercal$, A is similar to $-A$. This implies A and $-A$ have the same spectrum. Since λ is an eigenvalue of A if and only if $-\lambda$ is an eigenvalue of $-A$, we conclude that the adjacency spectrum of A is symmetric about 0. $\square$

In fact, our proof technique used in Proposition 5.1.2 can be used to prove a similar statement for the normalised Laplacian spectrum.

Proposition 5.1.2. Let G be a directed graph with *no isolated vertices*, then its normalised Laplacian spectrum of is symmetric about 1.

Proof. Recall that if G has no isolated vertices, we have $\mathcal{L} = I_n - D^{-1/2}AD^{-1/2}$. Applying similar analysis as in the proof of Proposition 5.1.2 on the matrix $D^{-1/2}AD^{-1/2}$ shows that the eigenvalues of $D^{-1/2}AD^{-1/2}$ is symmetric about 0. It follows that the eigenvalues of $\mathcal{L}$ is symmetric about 1. $\square$

This motivates us to define **spectral expansion** of a directed graph G as $\mu(G) = \max_{j\in\{1,\ldots n\}} |1-\mu_j| = 1-\mu_1$. In particular, for directed graph with no isolated vertices, we have $\mu(G) = 1-\mu_1 = \mu_n - 1$. For a directed graph G with isolated vertices, we know each trivial component of G contributes a 0 to the normalised Laplacian spectrum. In some sense, its normalised Laplacian spectrum is symmetric about 1 if we "ignore" these trivial 0's. Furthermore, it is possible that $\mu(G) = 1-\mu_1 = 1 > \mu_n - 1$.

5.2 Directed Graphs with maximum spectral expansion

We now revisit earlier studies on cospectrality for mixed graphs by restricting them to directed graphs. It is clear that a weakly connected directed graph $G = (V,E)$ has no isolated vertices. For *weakly connected directed graphs*, the following conditions are equivalent.

(i) G is cospectral to Γ_G.

(ii) $\lambda_1(G) = \lambda_1(\Gamma_G)$.

(iii) $\lambda_n(G) = -\lambda_1(\Gamma_G)$.

(iv) There exists a partition of V into 4 (possibly empty) parts V_1, V_i, V_{-1}, V_{-i} such that the following holds. Every edge of G is a directed edge from V_ω to $V_{-i\omega}$ for some $\omega \in \{1, i, -1, -i\}$. See Figure 5.1.

(v) G and Γ_G are switching equivalent.

(vi) G has the same Laplacian spectrum as Γ_G.

(vii) G has the same normalised Laplacian spectrum as Γ_G.

(viii) $\tau_1(G) = 0$.

(ix) $\mu_1(G) = 0$.

(x) $\mu_n(G) = 2$.

(xi) $\mu(G) = 1$.

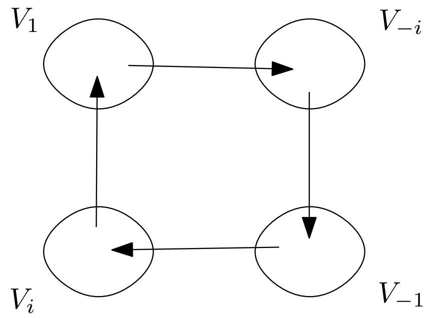


Figure 5.1: Structure for Directed Graphs with maximum spectral radius/expansion.

Note that if a directed graph G is not weakly connected, then conditions (ii), (iii), (viii), (ix), (x) and (xi) are necessary but not sufficient for G to be cospectral to its underlying graph Γ_G.

Observe that the equivalence of graph property based condition (iv) with other spectrum-based conditions has an interesting suggestion: the information about the flow of edges such as imbalances in the directions of the edges perhaps can be known by studying the various graph spectrum. We highlight an example which may arise naturally in many contexts: Suppose we are interested to investigate whether it's possible to partition the vertices of a directed graph $G = (V, E)$ into two partitions $V = V_1 \bigcup V_{-i}$ such that every edge is an edge from V_1 to V_{-i}, i.e. the net flow from V_1 to V_{-i} is exactly $|E|$. It follows that a necessary condition is that $\mu(G) = 1$.

We also remark that the example above can be seen as a directed analogue of the classic result in spectral theory of undirected graph: An undirected graph Γ can be partitioned into 2 components if and only if the *second* smallest eigenvalue of the normalised Laplacian matrix is 0 [Chu97, Lemma 1.7(iv)].

5.3 Directed Graphs with low spectral expansion

In the previous section, we have seen that having a maximum spectral expansion is necessary to be able to bi-partition a directed graph to achieve a net flow of $|E|$. In this section, we show that having a low spectral expansion corresponds to not being able to find *any* bi-partition that yields a high net flow.

Let $G = (V,E)$ be a directed graph. For any two subsets $S,T \subseteq V$, we define the net flow of edges from from S to T (counting edges contained in the intersection of S and T twice) as

$$\left|\left\{(v_1,v_2) \in S\times T : (v_1,v_2) \in E\right\}\right| - \left|\left\{(v_1,v_2) \in T\times S : (v_1,v_2) \in E\right\}\right|.$$

For ease of notation, we denote net flow of edges from from S to T as $\mathrm{Net}(S,T)$. We further denote $\mathrm{Vol}(S)$ as the sum of degree of the vertices in subset S.

The next theorem shows that for directed graphs with no isolated vertices, having a low spectral expansion corresponds to having a low $\mathrm{Net}(S,T)$ for *any* two subsets of vertices $S,T \subseteq V$. As a corollary, low spectral expansion corresponds to having a low net flow for *any* bi-partition of V.

Theorem 5.3.1. Let $G = (V,E)$ be a directed graph with no isolated vertices. Then, for any subsets $S,T \subseteq V$, we have

$$|\mathrm{Net}(S,T)| \le \mu(G)\sqrt{\mathrm{Vol}(S)\mathrm{Vol}(T)}$$

Proof. We write $\mathbf{1}_S$ as the column vector with k^{th} element being 1 if $v_k \in S$ and 0 otherwise. We define $\mathbf{1}_T$ similarly.

We first observe that

$$\begin{aligned}
-i\left(\mathbf{1}_S^\intercal A\mathbf{1}_T\right) &= -i\sum_{k=1}^{n}\sum_{j=1}^{n}\mathbf{1}_S A_{kj}\mathbf{1}_T \\
&= -i\left(\sum_{\substack{v_k\to v_j,\\ v_k\in S, v_j\in T}} i \quad + \sum_{\substack{v_j\to v_k,\\ v_k\in S, v_j\in T}} -i\right) \\
&= \left|\left\{(v_1,v_2) \in S\times T : (v_1,v_2) \in E\right\}\right| - \left|\left\{(v_1,v_2) \in T\times S : (v_1,v_2) \in E\right\}\right| \\
&= \mathrm{Net}(S,T)
\end{aligned}$$

Since G has no isolated vertices, we have $A = D^{1/2}(I_n - \mathcal{L})D^{1/2}$. Thus,

$$\begin{aligned}
\mathrm{Net}(S,T) &= -i\left(\mathbf{1}_S^\intercal\big(D^{1/2}(I_n-\mathcal{L})D^{1/2}\big)\mathbf{1}_T\right) \\
&= -i\left(\left(D^{1/2}\mathbf{1}_S\right)^\intercal(I_n-\mathcal{L})\left(D^{1/2}\mathbf{1}_T\right)\right)
\end{aligned}$$

Let $\{\mu_j\}_{j=1}^n$ be the eigenvalues of $\mathcal{L}$ and $\{f_j\}_{j=1}^n$ be the associated orthonormal eigenvectors. In particular, $f_k^\intercal f_j = 1$ if $k = j$ and 0 otherwise. Without loss of generality, we have

$$D^{1/2}\mathbf{1}_S = \sum_{j=1}^n a_j f_j$$

and

$$D^{1/2}\mathbf{1}_T = \sum_{k=1}^n b_k f_k$$

This implies

$$\begin{aligned}
|\mathrm{Net}(S,T)| &= \left| \Big(\sum_{j=1}^n a_j f_j \Big)^\intercal (I_n - \mathcal{L}) \Big(\sum_{k=1}^n b_k f_k \Big) \right| \\
&= \left| \Big(\sum_{j=1}^n \sum_{k=1}^n a_j b_k f_j^\intercal f_k \Big) - \Big(\sum_{j=1}^n \sum_{k=1}^n a_j b_k f_j^\intercal \mathcal{L} f_k \Big) \right| \\
&= \left| \Big(\sum_{j=1}^n a_j b_j \Big) - \Big(\sum_{j=1}^n a_j b_j f_j^\intercal \mu_j f_j \Big) \right| \\
&= \left| \Big(\sum_{j=1}^n (1-\mu_j)\, a_j b_j \Big) \right| \\
&\le \sum_{j=1}^n \Big| (1-\mu_j) \Big| \Big|\, a_j b_j \Big| \\
&\le \mu(G) \sum_{j=1}^n \Big|\, a_j b_j \Big| \\
&\le \mu(G) \sqrt{\sum_{j=1}^n a_j^2} \sqrt{\sum_{j=1}^n b_j^2} \\
&= \mu(G) \sqrt{\mathrm{Vol}(S)\mathrm{Vol}(T)}
\end{aligned}$$

where the first inequality follows from triangle inequality, the second inequality follows from the definition of spectral expansion, the third inequality follows from Cauchy-Schwarz inequality and the final equality follows from

$$\begin{aligned}
\sum_{j=1}^n a_j^2 &= \Big(\sum_{j=1}^n a_j f_j^\intercal \Big) \Big(\sum_{k=1}^n a_k f_k \Big) \\
&= (D^{1/2}\mathbf{1}_S)^\intercal D^{1/2}\mathbf{1}_S \\
&= \mathbf{1}_S^\intercal D \mathbf{1}_S \\
&= \sum_{v_j \in S} d(v_j) \\
&= \mathrm{Vol}(S).
\end{aligned}$$

□

We remark that the theorem above and its proof technique is similar to the well-studied Expander Mixing Lemma in the undirected settings [Chu97, Theorem 5.1].

Consider now a directed graph G with some isolated vertices. Notice that for any $S,T \subset V$, the isolated vertices in S and T does not contribute to any of the quantities $\mathrm{Net}(S,T)$, $\mathrm{Vol}(S)$, $\mathrm{Vol}(T)$. Hence, we can apply Theorem 5.3.1 on the induced sub-directed graph which leave out isolated vertices. We should also change the factor from $\mu(G)$ to $\mu_n - 1$, so that it corresponds to induced sub-directed graph which leave out isolated vertices. This gives us the following theorem.

Theorem 5.3.2. Let $G = (V,E)$ be a directed graph. Then, for any subsets $S,T \subseteq V$, we have

$$|\mathrm{Net}(S,T)| \leq (\mu_n - 1)\sqrt{\mathrm{Vol}(S)\mathrm{Vol}(T)}$$

5.4 (Quasi-)Random Oriented Graph

Theorem 5.3.2 says that for a directed graph G with a low μ_n, *any* two subsets $S,T \subseteq V(G)$ has a low $\mathrm{Net}(S,T)$. An intuitive interpretation of this phenomenon is that low spectral expansion corresponds to randomness (no clear structure of flow of edges) while high spectral expansion corresponds to structure (with extreme case having direction of edges as in Figure 5.1). In this section, we formalise this idea and give a brief discussion.

Let $\Gamma = (V,E)$ be an undirected graph. For convenience, we denote $\vec{\mathcal{D}}(\Gamma)$ to be the set of directed graphs with underlying graph being Γ. Consider generating a directed graph G from Γ by "randomly" assigning orientation to any $\{v_j, v_k\} \in E$ with probability 1/2 being $v_j \to v_k$ and probability 1/2 being $v_k \to v_j$.

It may happen that for certain graph properties $\mathcal{P}$, we have any randomly oriented directed graph $G \in \vec{\mathcal{D}}(\Gamma)$ satisfies $\mathcal{P}$ with high probability. In [Gri12, Theorem 1.1], it's proven that a number of conditions on directed graphs, all of which are satisfied with high probability by randomly oriented graphs, are in fact qualitatively equivalent. We call these conditions **quasi-randomness** conditions. We will state two of these conditions below, which are most relevant to our studies thus far.

Theorem 5.4.1. [Gri12, Theorem 1.1] The following conditions on a directed graph G are equivalent, in the sense that any one of them, with any positive value of its parameter can be deduced from the other, when the parameter of the latter is taken sufficiently small.

(i) $\mathrm{Net}(S,T) \leq \alpha n^2 \quad$ for all $\; S,T \subseteq V$.

(ii) $\lambda_1(G) \leq \beta n$.

We remark that Theorem 5.4.1 uses the spectral radius/biggest adjacency eigenvalue to capture the notion of "randomness" as compared to Theorem 5.3.2 which uses $\mu_n - 1$.

5.5 Upper bound for minimum Spectral Radius

Having studied the correspondence between low spectral radius and quasirandomness, it is natural to ask what is the minimum spectral radius taken over all possible orientations of a fixed underlying graph. We know from the discussion immediately after Proposition 3.3.4 that the directed graph K_4' with spectral radius of $\sqrt{3}$ in Figure 3.4 is such an example. For a general fixed underlying graph, [GMO19, Theorem 1.1] gives an upper bound for this value. The proof of this theorem uses the technique of interlacing families of polynomials. [1]

Before stating the theorem, we first recall the definition of matching polynomial for an undirected graph. Let m_k be the number of k-edge matchings of undirected graph Γ. We set $m_0 = 1$. The matching polynomial of Γ is defined as

$$M_\Gamma(x) := \sum_{k=0}^{n/2} (-1)^k m_k x^{n-2k}.$$

It is known for any undirected graph Γ, M_Γ is real rooted [God81]. Denote $\rho(M_\Gamma)$ as the biggest root of M_Γ. For more details about matching polynomial, see [EM11, Section 10.3.1]. We are now ready to state Theorem 1.1. of [GMO19].

Theorem 5.5.1. [GMO19, Theorem 1.1] Let Γ be an undirected graph and let M_Γ be its matching polynomial. Then there exists an orientation σ of Γ such that the directed graph $G \in \vec{\mathcal{D}}(\Gamma)$ with orientation σ satisfies $\lambda_1(G) \leq \rho(M_\Gamma)$.

It is known that for any undirected graph Γ, $\rho(M_\Gamma) \leq \lambda_1(\Gamma)$. If Γ is connected then $\rho(M_\Gamma) = \lambda_1(\Gamma)$ if and only if Γ is a tree [GG81]. Recall from Corollary 4.1.5 that for an undirected tree T (a special case of forest), all directed graphs (special case of mixed graphs) whose underlying graph is T are cospectral with T. Hence, we see that for a tree T, any $G \in \vec{\mathcal{D}}(T)$ has $\lambda_1(G) = \rho(M_T) = \lambda_1(T)$. Therefore, Theorem 5.5.1 is tight.

[1] This method is first used in the seminal paper [MSS15] to prove the existence of infinite families of Ramanujan graphs.

Chapter 6

Conclusion

In this project, we have surveyed existing results for Hermitian adjacency, Hermitian Laplacian and normalised Hermitian Laplacian matrix of mixed graphs simultaenously. In particular, we highlighted if certain results have an analogue in the undirected setting, as well as the similarity in the proof technique used. Along the way, we proved some new results. Perhaps the most interesting result is that we know how to construct non-isomorphic mixed graphs which are cospectral with respect to all three matrix representations (See Chapter 4.1). We also provided new proof for Theorem 3.3.1 and Proposition 5.1.2.

Future Work

In the undirected settings, near-zero normalised Laplacian eigenvalues have found applications in spectral clustering [Lux07, Section 7]. This corresponds to "structure". Meanwhile, having *second* largest eigenvalue that is far from the first is basically what characterises an expander graph. This corresponds to the "randomness" [Alo86].

It is interesting to investigate if analogous studies can be done for directed graphs through spectral radius and spectral expansion. In particular, we know there are results (though the intention of study was for graph energy) showing for all positive integers d, there exists a d-regular graph with orientations having the theoretical minimum spectral radius of $\sqrt{d}$ [Tia11]. In fact, we know how to recursively construct them. This result, together with [GMO19] makes the situation somewhat looks like the study of expander and Ramanujan graph in the undirected settings. The author believes that this is a promising direction of research which could potentially comparable to expander graph.

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