THE NORMALIZED LAPLACIAN MATRIX AND GENERAL RANDIĆ INDEX OF GRAPHS

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Abstract

To any graph we may associate a matrix which records information about its structure. The goal of spectral graph theory is to see how the eigenvalues of such a matrix representation relate to the structure of a graph.

In this thesis, we focus on a particular matrix representation of a graph, called the normalized Laplacian matrix, which is defined as $\mathcal{L} = D^{-1/2}(D - A)D^{-1/2}$, where D is the diagonal matrix of degrees and A is the adjacency matrix of a graph. We first discuss some basic properties about the spectrum and the largest eigenvalue of the normalized Laplacian. We study graphs that are cospectral with respect to the normalized Laplacian eigenvalues. Properties of graphs with few normalized Laplacian eigenvalues are discussed. We then investigate the relationship that the normalized Laplacian eigenvalues have to the general Randić index $R_{-1}(G)$ of a graph, defined as $R_{-1}(G) = \sum_{x \sim y} \frac{1}{d_x d_y}$, where d_x is the degree of the vertex x.

We next consider the energy of a simple graph with respect to its normalized Laplacian eigenvalues, which we call the $\mathcal{L}$-energy. The $\mathcal{L}$-energy of a graph G is $E_{\mathcal{L}}(G) = \sum_{i=1}^{n} |\lambda_i(\mathcal{L}) - 1|$, where $\lambda_1(\mathcal{L}), \ldots, \lambda_n(\mathcal{L})$ are the eigenvalues of $\mathcal{L}$.

Over graphs of order n that contain no isolated vertices, we characterize the graphs with minimal $\mathcal{L}$-energy of 2 and maximal $\mathcal{L}$-energy of $2\lfloor n/2 \rfloor$. The graphs of maximal $\mathcal{L}$-energy are disconnected, which leads to the question: "What are the connected graphs of order n that have the maximum $\mathcal{L}$-energy?"

The technique we use is to first bound the $\mathcal{L}$-energy of a graph G in terms of its general Randić index $R_{-1}(G)$. We highlight known results for $R_{-1}(G)$, most of which assume that G is a tree. We extend an upper bound on $R_{-1}(G)$ from trees to connected graphs, which in turn, provides a bound on the $\mathcal{L}$-energy of a connected graph. We conjecture that the maximal $\mathcal{L}$-energy of a connected graph is equal to $\frac{n}{\sqrt{2}}$ asymptotically and provide a class of graphs with this property.

We also discuss the maximum change of $\mathcal{L}$-energy and $R_{-1}(G)$ upon edge deletion. Finally, we provide bounds on the $\mathcal{L}$-energy in terms of other parameters, one of which is the energy with respect to the adjacency matrix eigenvalues.

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Post Defense Acknowledgement

Besides my advisors, I would like to thank the rest of my thesis committee. This includes Cory Butz, Allen Herman and Karen Meagher. I would also like to give a special thanks to my External Examiner Sebastian Cioabă for his helpful remarks. Finally, I'd like to acknowledge Nader Mobed, who acted as Chair of my oral defense.

Dedication

I would like to dedicate this thesis to my family and friends.

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1 SPECTRAL GRAPH THEORY

1.1 Introduction to spectral graph theory

The foundations of spectral graph theory were laid in the 1950's and 1960's, however, its origins can be traced back even earlier. In quantum chemistry, the ideas of spectral graph theory can be found in a 1931 paper of Hückel [37] where eigenvalues of graphs are used to represent the levels of energy of certain electrons. The well-known Matrix-Tree Theorem (for example, see [17]) can be thought of as a result in spectral graph theory and was proved by Brooks, Smith, Stone and Tutte [7] in 1940 and independently by Trent [63] in 1954. Many authors hold that the Matrix-Tree Theorem is implicitly contained in Kirchhoff's classic 1847 paper [39] (for more details consult [49, Chapter 5]).

Since the fundamental paper of Collatz and Sinogowitz [15] in 1957, spectral graph theory has appeared frequently in the mathematical literature. In [15], the authors obtain a connection between the degrees of a graph and eigenvalues and make further observations regarding graph spectra. Even earlier, Cvetković, Rowlinson and Simić [18] claim that the investigation between spectral and structural properties of graphs can be found in the unpublished thesis of Wei [66] from 1952 and an unpublished summary of a 1956 paper by Lihtenbaum [44] communicated at the 3rd Congress of Mathematicians of the U.S.S.R. Since then, spectral graph theory has been well documented in several surveys and books (for example, see [2, 3, 8, 16, 17, 18, 27, 60]).

The general idea in spectral graph theory is that to any graph we may associate a corresponding matrix which records information about its structure. The fundamental problem in spectral graph theory is to answer the following question:

Question 1.1.1 *How do the eigenvalues of a matrix representation of a graph relate to the structure of the graph?*

Thus, when studying spectral graph theory, one needs to be familiar with both graph theory and tools of linear algebra.

In Chapter 1, we first give a brief overview of the notation, terminology and key results from graph theory and matrix theory that will be used throughout this thesis. We then investigate notions of the *energy* of a graph and the *general Randić index* of a graph.

In Chapter 2, we turn our focus to the normalized Laplacian matrix and discuss the importance of the largest eigenvalue. Using Godsil-McKay switching, it is shown how to construct cospectral graphs with respect to the normalized Laplacian eigenvalues. We discuss properties of graphs with two or three distinct normalized Laplacian eigenvalues. We emphasize the relationship that the general Randić index has with the spectrum of the normalized Laplacian. Then we highlight and rephrase results developed by Runge (in the 1970's) in terms of $\mathcal{L}$, which includes a Matrix-Tree Theorem and Coefficients Theorem for $\mathcal{L}$.

In Chapter 3, we discuss bounds on the general Randić index of a graph. Upper and lower bounds are given in terms of the order of a graph, as well as the minimum and maximum degrees. These bounds can be improved when restricted to the class of connected graphs. We then look at the effect edge deletion has on the general Randić index.

In Chapter 4, we consider the energy of a graph with respect to its normalized Laplacian eigenvalues, which we call the $\mathcal{L}$-energy. Over graphs of order n that contain no isolated vertices, we characterize the graphs with minimal and maximal $\mathcal{L}$-energy, and discuss the maximal $\mathcal{L}$-energy over the class of connected graphs. We provide bounds on the $\mathcal{L}$-energy in terms of other parameters, one of which is the energy with respect to the adjacency matrix. Finally, we look at the effect edge deletion has on the $\mathcal{L}$-energy. We provide examples to show that both $\mathcal{L}$-energy and the general Randić index can decrease, stay the same or increase upon edge deletion.

Lastly, in Chapter 5, we summarize and discuss some open problems and future considerations.

Note that the results from Chapters 3 and 4 have been published in [11]. It should also be mentioned that recent results on the normalized Laplacian energy have also appeared in [6] under the name of Randić energy.

1.2 Graph theory: Notation, definitions and key results

A paper written on the *Seven Bridges of Königsberg* problem, published by Euler in 1736, is regarded as the first paper in the field of graph theory [3]. Briefly, the problem is to find a walk through the city of Königsberg (see Figure 1.1) that would cross each bridge exactly once. Euler showed that the problem has no solution. He noted that if every bridge is traversed exactly once then the number of bridges touching each land mass must be even (except possibly for the land masses chosen for the start and finish). By noting that all four land masses in Figure 1.1 are touched by an odd number of bridges and since at most two land masses can serve as the endpoints of a walk, the existence of a walk traversing each bridge exactly once leads to a contradiction. Euler's solution of the Seven Bridges of Königsberg problem laid the foundations of graph theory and led to the concept of Eulerian graphs.

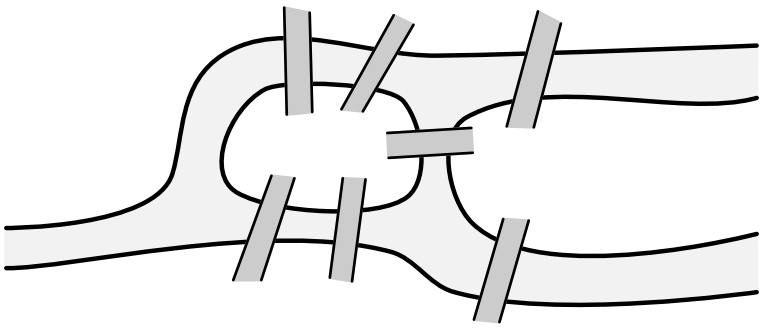

Figure 1.1: Depiction of Königsberg highlighting the Pregel river and the layout of the seven bridges.

The applications of graph theory reach far and wide. It is used in communication networks, computer science, physics, biology, chemistry, sociology and many other fields. In this section we will go through the basic terminology and notation that will be used in this thesis (for more details, see [3, 17, 23]).

A *graph*, denoted by G, is a pair (V, E) of sets such that the elements of E are a collection of 2-element subsets of V. We call the elements of V the *vertices* of the graph, and the elements of E the *edges* of the graph. We use the notation xy to denote an edge $\{x, y\}$, for distinct $x, y \in V$. The number of vertices $|V|$ of a graph G is its *order*. We often use the phrase *a graph on n vertices* to mean that the graph has order n, and similarly, the phrase

a graph with m edges to mean that $|E| = m$.

Typically, a graph is pictured as a set of dots (which corresponds to the vertices), with some pairs of dots joined by lines (with each line corresponding to an edge). In Figure 1.2 a graph with vertex set $V = \{1, 2, 3, 4, 5, 6\}$ and edge set $E = \{12, 15, 23, 24, 25, 36, 45, 56\}$ is illustrated.

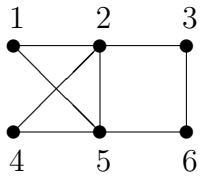

Figure 1.2: An example of a graph on 6 vertices.

If $e = xy$ is an edge of G, then we say vertex x is *incident* with e, and that e is an edge *at* x. The two vertices incident with an edge are called its *endpoints*. Two vertices x, y of G are *adjacent*, if xy is an edge of G. We often use the notation $x \sim y$ to mean that x is adjacent to y in G. Similarly, two edges e, f of G are *adjacent*, if they have an endpoint in common. A set of vertices (or edges) is called *independent* if no two elements of the set are adjacent. If xy is an edge of G, we say y is a *neighbour* of x. We denote the set of neighbours of x by N_x.

Let $G = (V, E)$ and $G' = (V', E')$ be two graphs. We call G and G' *isomorphic* if there is a bijection $\phi : V \to V'$ with $xy \in E$ if and only if $\phi(x)\phi(y) \in E'$, for all $x, y \in V$. We usually do not distinguish between isomorphic graphs in the sense that relabeling the vertices of a graph gives the "same" graph. The term *graph* in this thesis refers to an unlabeled graph in the sense that individual vertices have no distinct identifications except through their interconnectivity. If $V' \subseteq V$ and $E' \subseteq E$, then we call G' a *subgraph* of G. Further, G' is an *induced subgraph* of G if G' is a subgraph of G and G' contains *all* the edges $xy \in E$ with $x, y \in V'$. If G' is a subgraph of G with $V' = V$ then we say G' is a *spanning* subgraph of G.

Let S be a subset of vertices of V. We denote the graph obtained by deleting all the vertices in S and their incident edges by $G \backslash S$. If e is an edge of G, we denote by $G - e$ the graph obtained by removing the edge e from G. The *complement* $\bar{G}$ of a graph G is the graph with the same vertex set as G, where any two distinct vertices are adjacent if and only if they are non-adjacent in G.

The *degree* of a vertex x of G, denoted d_x, is the number of edges at x. If there is more than one graph in question, we write d_x^G to denote the degree of x in G. A vertex of degree

0 is called an *isolated* vertex. The number $d_{\min} = \min\{d_x | x \in V\}$ is called the *minimum degree* of G, while the number $d_{\max} = \max\{d_x | x \in V\}$ is called the *maximum degree* of G. If each vertex has the same degree r, then G is called an *r-regular* graph, or simply, a *regular* graph. A simple observation is that the number of edges in a graph can be expressed as

$$|E(G)| = \frac{1}{2} \sum_{x \in V} d_x.$$

A graph on n vertices that is regular of degree $n-1$ is called the *complete graph* and is denoted by K_n. Illustrated in Figure 1.3 are the complete graphs with 3, 4 and 5 vertices.

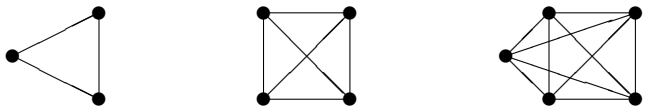

Figure 1.3: The complete graphs on 3, 4 and 5 vertices.

A *walk* in a graph $G = (V, E)$ is a sequence of vertices $\{x_1, x_2, \ldots, x_t\}$ with $x_i x_{i+1} \in E$ for all $1 \leq i \leq t-1$, where repetition is allowed amongst the x_i's. A *path* on n vertices is a graph (V, E) with vertex set $V = \{x_1, x_2, \ldots, x_n\}$ and edge set

$$E = \{x_1x_2, x_2x_3, \ldots, x_{n-1}x_n\},$$

where the x_i are all distinct. The number of edges of a path is its *length*. A path of length k is commonly denoted by P_k and has $k+1$ vertices. We often denote a path as $P = x_1x_2 \ldots x_n$ and say P is a path *from x_1 to x_n*. If a path P_k from x_r to x_s is a subgraph of G then we say G *contains* a path of length k from x_r to x_s. Illustrated in Figure 1.4 is a path of length $n-1$.

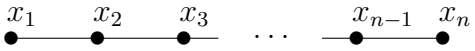

Figure 1.4: A path on n vertices.

The *distance* between two vertices x, y in G, denoted $dist(x, y)$, is the length of a shortest path from x to y in G (if no such path exists we set $dist(x, y) = \infty$). The greatest distance between any pair of vertices in G is called the *diameter* of G and is denoted by $diam(G)$.

A *cycle* on n vertices is a graph with vertex set $V = \{x_1, x_2, \ldots, x_n\}$ and edge set $E = \{x_1x_2, x_2x_3, \ldots, x_{n-1}x_n, x_nx_1\}$, where the x_i are all distinct. The number of edges of a

cycle is its *length*. A cycle of length k is commonly denoted by C_k and has k vertices and k edges. A cycle of odd length is called an *odd cycle*. If a cycle C_k is a subgraph of G then we say G *contains* a cycle of length k. Illustrated in Figure 1.5 are the cycles on 3, 4 and 5 vertices.

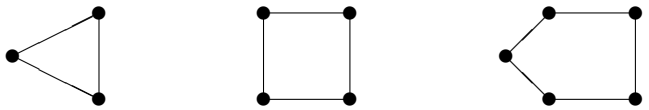

Figure 1.5: The cycle graphs on 3, 4 and 5 vertices.

A graph G is called *connected* if between any pair of vertices x, y of G, there is a path contained in G between x and y. On the other hand, if there is a pair of vertices x, y of G such that no path between x and y exists in G, we say G is *disconnected*. A maximal connected subgraph of G is called a *component* of G.

A connected graph that does not contain any cycles is called a *tree*. A graph whose components are all trees is called a *forest*. Let G be a graph (not necessarily a tree), then we call a vertex of degree 1 a *leaf*. An edge incident to a leaf is a *leaf edge*. An edge not incident to any leaf is a *non-leaf edge*. Every tree has at least two leaf edges. If a tree on n vertices has $n - 1$ leaves, then this tree is called a *star*. The star graphs on 4, 5 and 6 vertices are illustrated in Figure 1.6. Every graph that is a star or a path is also a tree since they do not contain any cycles.

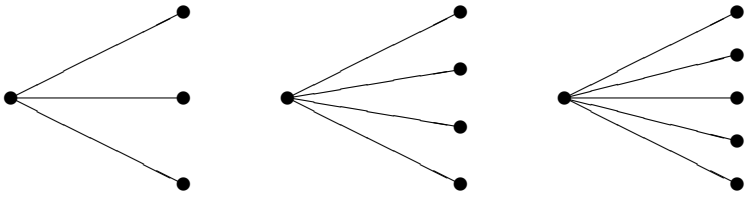

Figure 1.6: Star graphs on 4, 5 and 6 vertices.

Let $k \geq 2$ be an integer. A graph is called *k-partite* if its vertices can be partitioned into k disjoint sets so that no two vertices within the same set are adjacent. When $k = 2$, we often call a 2-partite graph a *bipartite* graph. The partition classes of a k-partite graph are called its *parts*. If in a k-partite graph, every pair of vertices from different parts are adjacent, then the graph is called *complete k-partite*. The collection of all complete k-partite

graphs (for all k) is referred to as the class of *complete multipartite graphs*. The complete k-partite graph whose parts have sizes $n_1, n_2, \ldots, n_k$ is denoted by $K_{n_1,n_2,\ldots,n_k}$. A star graph on n vertices can be thought of as a complete bipartite graph with two parts of sizes 1 and $n-1$, and hence is denoted by $K_{1,n-1}$. The *center* of a star is the vertex in the part of size 1 of $K_{1,n-1}$. The complete bipartite graph $K_{3,5}$ is illustrated in Figure 1.7.

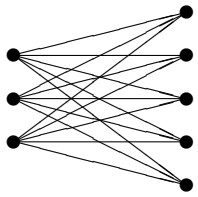

Figure 1.7: The complete bipartite graph $K_{3,5}$.

A k-partite graph is called *semiregular* if any two vertices in the same colour class have the same degree. For example, the complete bipartite graph $K_{p,q}$ is semiregular as each vertex in the part with size p has degree q, and each vertex in the part of size q has degree p. Bipartite graphs cannot contain an odd cycle and are characterized by this property.

Theorem 1.2.1 *[23, Proposition* 1.6.1*] A graph is bipartite if and only if it contains no odd cycles.*

We next list two ways to construct graphs from two given graphs. The *union* of two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, with disjoint vertex sets V_1 and V_2, is the graph denoted $G_1 \cup G_2$ with vertex set $V_1 \cup V_2$ and edge set $E_1 \cup E_2$. See Figure 1.8 for an example of the union of two graphs. The graph denoted by sG is s disjoint copies of the graph G where we assume each copy of G has a distinct vertex set from every other copy, that is, $sG = \bigcup_{i=1}^{s} G$.

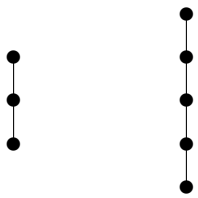

Figure 1.8: The graph union of the paths P_2 and P_4, that is, $P_2 \cup P_4$.

The *join* of two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, with disjoint vertex sets V_1 and V_2, is the graph denoted $G_1 \vee G_2$ with vertex set $V_1 \cup V_2$ and edge set

$$E_1 \cup E_2 \cup \{x_1x_2 : x_1 \in V_1, x_2 \in V_2\}.$$

See Figure 1.9 for an example of the join of two graphs.

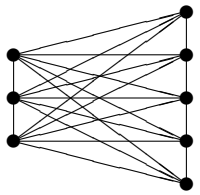

Figure 1.9: The graph join of the paths P_2 and P_4, that is, $P_2 \vee P_4$.

It should be noted that there are other notions of graphs, such as, multigraphs, directed graphs and hypergraphs. In this thesis, we will concentrate on *simple* graphs, in the sense that each pair of vertices either has exactly 1 or 0 (undirected) edges between them, and that no vertex has an edge going to itself. When analyzing the general Randić index of a graph, defined later in Section 1.9, we will deal with weighted graphs, where each edge (or vertex) of a graph is given a numerical value, called its *weight*.

1.3 Matrix representations of graphs

Given a graph G, we can form a matrix that contains information about the structure of the graph. Some of the most commonly studied matrix representations of graphs are the adjacency matrix, combinatorial Laplacian, signless Laplacian and the normalized Laplacian.

The *adjacency matrix* of a graph $G = (V, E)$, denoted by A, is a matrix whose rows and columns are indexed by the vertices of G, and is defined to have entries

$$A(x, y) = \begin{cases} 1 & \text{if } xy \in E, \\ 0 & \text{otherwise.} \end{cases}$$

The *combinatorial Laplacian* of a graph $G = (V, E)$, denoted by L, is a matrix whose rows and columns are indexed by the vertices of G, and is defined to have entries

$$L(x, y) = \begin{cases} d_x & \text{if } x = y, \\ -1 & \text{if } xy \in E, \\ 0 & \text{otherwise.} \end{cases}$$

This matrix is closely related to the adjacency matrix A of G. Let D be a diagonal matrix, whose rows and columns are indexed by the vertices of G, with diagonal entries $D(x,x) = d_x$. Then,

$$L = D - A.$$

The matrix $D + A$ is called the *signless Laplacian* of a graph and is denoted by $|L|$. It should be noted that the signless Laplacian is sometimes denoted by L^+ or Q in the literature, however, we will use Q to denote $D^{-1}A$ in this thesis to match the notation in [17]. Finally, the *normalized Laplacian* of a graph $G = (V, E)$, denoted by $\mathcal{L}$, is a matrix whose rows and columns are indexed by the vertices of G, and is defined to have entries

$$\mathcal{L}(x,y) = \begin{cases} 1 & \text{if } x = y \text{ and } d_y \neq 0, \\ -\dfrac{1}{\sqrt{d_x d_y}} & \text{if } xy \in E, \\ 0 & \text{otherwise.} \end{cases}$$

We discuss the normalized Laplacian matrix in more detail in Chapter 2.

As an illustration, we list the four matrix representations defined above for the graph in Figure 1.2 (using the labeling $\{1,2,3,4,5,6\}$ of the vertices to index the rows and columns of the matrices):

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}, \quad L = \begin{bmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 4 & -1 & -1 & -1 & 0 \\ 0 & -1 & 2 & 0 & 0 & -1 \\ 0 & -1 & 0 & 2 & -1 & 0 \\ -1 & -1 & 0 & -1 & 4 & -1 \\ 0 & 0 & -1 & 0 & -1 & 2 \end{bmatrix},$$

$$|L| = \begin{bmatrix} 2 & 1 & 0 & 0 & 1 & 0 \\ 1 & 4 & 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 0 & 0 & 1 \\ 0 & 1 & 0 & 2 & 1 & 0 \\ 1 & 1 & 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 0 & 1 & 2 \end{bmatrix}, \quad \mathcal{L} = \begin{bmatrix} 1 & -\frac{1}{\sqrt{8}} & 0 & 0 & -\frac{1}{\sqrt{8}} & 0 \\ -\frac{1}{\sqrt{8}} & 1 & -\frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & -\frac{1}{4} & 0 \\ 0 & -\frac{1}{\sqrt{8}} & 1 & 0 & 0 & -\frac{1}{2} \\ 0 & -\frac{1}{\sqrt{8}} & 0 & 1 & -\frac{1}{\sqrt{8}} & 0 \\ -\frac{1}{\sqrt{8}} & -\frac{1}{4} & 0 & -\frac{1}{\sqrt{8}} & 1 & -\frac{1}{\sqrt{8}} \\ 0 & 0 & -\frac{1}{2} & 0 & -\frac{1}{\sqrt{8}} & 1 \end{bmatrix}.$$

1.4 Linear algebra: Notation, definitions and key results

In this section we give some background information and list the basic tools of linear algebra that will be used in this thesis (for more details, see [17, 36]). We use the notation I_n for the identity matrix of order n, $J_{m\times n}$ for the $m \times n$ matrix where each entry is equal to 1, $\mathbf{1}_n$ for the vector of length n consisting of all ones, $\mathbf{0}_{m\times n}$ for the $m \times n$ zero matrix, and $\mathbf{0}_n$ for the zero vector of length n. We often ignore the subscripts when the size of the matrix is clear from the context. A permutation matrix, usually denoted P, is a square matrix that has exactly one entry consisting of a 1 in each row and each column, and 0's elsewhere.

Let M be a real matrix of order n. The notation M^T is used for the transpose of M. The *eigenvalues* of M can be defined as the numbers λ satisfying $Mx = \lambda x$ for a non-zero vector x. Each such vector x is called an *eigenvector* of the matrix M belonging to the eigenvalue λ. The *spectrum* of a matrix is the set of its eigenvalues together with their multiplicities (although it is more correct to say we are dealing with a multiset). Alternatively, one can define the eigenvalues as being the zeros of the *characteristic polynomial* of M, that is, the zeros of $\det(\lambda I - M)$. The *singular values* of M can be defined as the numbers σ satisfying $Mv = \sigma u$ and $M^T u = \sigma v$ for two non-zero vectors u and v.

The set of eigenvectors belonging to an eigenvalue λ along with the zero vector forms the *eigenspace belonging to* λ. The *geometric multiplicity of* λ is the dimension of its eigenspace. The *algebraic multiplicity of* λ is the multiplicity of λ considered as a zero of the corresponding characteristic polynomial. In general, the algebraic multiplicity of λ is greater than or equal to the geometric multiplicity of λ (see [36]).

The well-known *Cayley-Hamilton Theorem* (for example, see [36]) says that each square matrix M satisfies its own characteristic polynomial, that is, if $f(\lambda) = \det(\lambda I - M)$, then $f(M) = \mathbf{0}$. The *minimal polynomial* $m(\lambda)$ of M is the monic polynomial of degree k such that k is minimal under the condition $m(M) = \mathbf{0}$. It is known that (for example, see [17]):

- $m(\lambda)$ is uniquely determined by M.
- If $F(\lambda)$ is any polynomial with $F(M) = \mathbf{0}$, then $m(\lambda)|F(\lambda)$.
- If $\{\mu_1, \ldots, \mu_p\}$ are the distinct eigenvalues of M such that μ_i has algebraic multiplicity m_i, then
$$\det(\lambda I - M) = (\lambda - \mu_1)^{m_1} \cdots (\lambda - \mu_p)^{m_p},$$

and

$$m(\lambda) = (\lambda - \mu_1)^{q_1} \cdots (\lambda - \mu_p)^{q_p},$$

for some $0 < q_i \leq m_i$, $1 \leq i \leq p$.

A matrix M is called *symmetric* if $M^T = M$. Two vectors x and y of the same length are *orthogonal* to each other, written as $x \perp y$, if $y^T x = 0$. A set of vectors $\{x_1, \ldots, x_n\}$ form an *orthonormal* set if each pair of vectors are orthogonal to each other and $x_i^T x_i = 1$ for each i. Some of the key results about the eigenvalues of symmetric matrices are the following (for example, see [17, 36]).

Theorem 1.4.1 *[17, 36] Let M be a real symmetric matrix of order n. Then the following hold:*

(i) The eigenvalues of M are real numbers.

(ii) The geometric and algebraic multiplicities of any eigenvalue of M are equal.

(iii) The singular values of M are the absolute values of its eigenvalues.

(iv) The eigenvectors of M can be chosen to be orthogonal to each other. In fact, they can be chosen to form an orthonormal basis of $\mathbb{R}^n$.

If M is a square matrix of order n, we order and denote the singular values by

$$\sigma_1(M) \leq \ldots \leq \sigma_n(M).$$

The following theorem, first proven by Fan [24], is quite useful when dealing with singular values.

Theorem 1.4.2 *[24] Let A and B be square matrices of order n. Then*

$$\sum_{i=1}^{n} \sigma_i(A + B) \leq \sum_{i=1}^{n} \sigma_i(A) + \sum_{i=1}^{n} \sigma_i(B).$$

A real symmetric matrix M of order n is said to be *positive semidefinite*, if

$$x^T M x \geq 0,$$

for all $x \in \mathbb{R}^n$. A key result is the following characterizations of positive semidefinite matrices.

Theorem 1.4.3 *[36] Let M be a real symmetric matrix of order n. Then the following are equivalent:*

(i) M is positive semidefinite, that is, $x^T Mx \geq 0$, for all $x \in \mathbb{R}^n$.

(ii) All eigenvalues of M are nonnegative.

(iii) There exists a matrix S such that $M = SS^T$.

Each of the four matrix representations defined in Section 1.3 are real symmetric matrices, and hence by Theorem 1.4.1, their eigenvalues are real numbers and can be ordered. In this thesis, if M is a real symmetric matrix of order n, we order and denote the eigenvalues by

$$\lambda_1(M) \leq \ldots \leq \lambda_n(M).$$

It should be noted that other authors sometimes start with λ_0 instead of λ_1, or reverse the notation. When referring to the *multiplicity* of an eigenvalue, we mean the algebraic multiplicity. It is well known that the trace of a square matrix M (that is, the sum of the diagonal entries of M), denoted $tr(M)$, is equal to the sum of its eigenvalues:

$$tr(M) = \sum_{i=1}^{n} \lambda_i(M).$$

Note that if M is a matrix of order n, then for $a, b \in \mathbb{R}$, the eigenvalues of $aM + bI_n$ are

$$a\lambda_1(M) + b,\ a\lambda_2(M) + b, \ldots,\ a\lambda_n(M) + b.$$

We next discuss how the eigenvalues of two matrices can be related. A matrix B is said to be *similar* to a matrix C if there exists a nonsingular matrix S such that $B = SCS^{-1}$, where each of B, C and S are of order n. In the case that S is a permutation matrix then we say B and C are *permutation similar*. Note that a permutation matrix P satisfies $P^{-1} = P^T$. Similarity is an equivalence relation on the set of matrices of order n. The next important result says that similar matrices have the same spectrum.

Theorem 1.4.4 *[36, Corollary 1.3.4] If B and C are similar matrices, then they have the same eigenvalues, counting multiplicity.*

If B and C are not similar but instead satisfy the equation $B = SCS^T$, then two useful theorems relating their eigenvalues are *Sylvester's law of inertia* and another due to Ostrowski

(see [36, Theorem 4.5.9]), which we state for real symmetric matrices. The *inertia* of a real symmetric matrix M, denoted by $i(M)$, is the ordered triple (n_1, n_2, n_3), where n_1 (resp. n_2 and n_3) is the number of positive (resp. negative and zero) eigenvalues of M.

Theorem 1.4.5 *[36, Theorem 4.5.8] (Sylvester's law of inertia) Let B and C be real symmetric matrices of order n. There exists a nonsingular matrix S of order n such that $B = SCS^T$ if and only if $i(B) = i(C)$.*

Theorem 1.4.5 does not answer the question of how the magnitudes of the eigenvalues of two matrices relate to each other. The next theorem, given by Ostrowski, gives a quantitative form of Sylvester's law of inertia relating the eigenvalues of a matrix M with those of SMS^T, for some nonsingular matrix S. First note that if S is a matrix, then SS^T is a symmetric matrix.

Theorem 1.4.6 *[36, Theorem 4.5.9] Let M be a real symmetric matrix of order n and S a nonsingular matrix of order n. For each $k = 1, 2, \ldots, n$, there exists a positive real number θ_k such that*

$$\lambda_1(SS^T) \leq \theta_k \leq \lambda_n(SS^T)$$

and

$$\lambda_k(SMS^T) = \theta_k \lambda_k(M).$$

Consider the adjacency matrix A of a graph G. In some sense, the adjacency matrix is not unique as relabeling the vertices of the graph produces another adjacency matrix. This corresponds to simultaneously permuting the rows and columns of A. That is, there is a permutation matrix P such that the graph with its vertices relabeled has adjacency matrix PAP^T. Thus, for each graph G, there is a class $\mathcal{A}(G)$ of adjacency matrices, with two adjacency matrices A_1 and A_2 belonging to the same class if and only if A_1 and A_2 are permutation similar. Therefore, a graph G (and its isomorphic images) may be uniquely identified with its matrix class $\mathcal{A}(G)$. The eigenvalues of two adjacency matrices A_1 and A_2 belonging to the same class are the same by Theorem 1.4.4. The eigenvectors can also be thought of as being independent on the choice of labeling. This leads to the following important observation in spectral graph theory.

Observation 1.4.7 *[23] If two graphs are isomorphic then their adjacency matrices have the same spectrum.*

Let G be a graph with a matrix representation M. The *M-eigenvalues* of G are the eigenvalues of M together with their multiplicities. The *M-spectrum* of G is the multiset of M-eigenvalues of G. In the case of the adjacency matrix, we simply refer to the A-eigenvalues and A-spectrum as the eigenvalues of G and (ordinary) spectrum of G respectively.

The converse of Observation 1.4.7 is false, as there are non-isomorphic graphs that have the same spectrum. Observation 1.4.7 also holds for the M-spectrum where M is one of L, $|L|$ or $\mathcal{L}$, and the converse is also false for each of these matrix representations. If two graphs have the same M-spectrum then we say the two graphs are *cospectral with respect to the M-eigenvalues*. In Chapter 2, we construct examples of pairs of non-isomorphic cospectral graphs with respect to the four matrix representations listed in Section 1.3. The study of cospectral graphs is one of the most interesting and important problems in spectral graph theory (see [20, 21]).

There is a lot known about the A-eigenvalues of a graph (for example, see [2, 8, 16, 17, 18, 27]) and a lot of study has been done regarding the L-eigenvalues and $|L|$-eigenvalues of graphs. In Chapter 2 we discuss the spectrum of $\mathcal{L}$ in more detail.

1.5 Equitable partitions of matrices and graphs

Here we focus on a technique that can be used to compute some of the eigenvalues of a matrix by investigating a corresponding matrix of smaller order. Suppose A is a real symmetric matrix of order n whose rows and columns are indexed by $X = \{1, 2, \ldots, n\}$. Let $\{X_1, X_2, \ldots, X_r\}$ be a partition of X with each $X_i \neq \emptyset$. The *characteristic matrix* S is the $n \times r$ matrix whose jth column is the characteristic vector of X_j, for $j = 1, 2, \ldots, r$, that is,

$$S(i,j) = \begin{cases} 1 & \text{if } i \in X_j, \\ 0 & \text{otherwise.} \end{cases}$$

Let K be the diagonal matrix of order r whose (i,i)th entry is $|X_i|$. Then $S^T S = K$ and K is a nonsingular matrix as each X_i is nonempty.

Let A be partitioned according to $\{X_1, X_2, \ldots, X_r\}$, that is,

$$A = \begin{bmatrix} A_{1,1} & \cdots & A_{1,r} \\ \vdots & & \vdots \\ A_{r,1} & \cdots & A_{r,r} \end{bmatrix},$$

where $A_{i,j}$, called a *block* of A, denotes the submatrix of A formed by rows in X_i and columns in X_j. Let $b_{i,j}$ denote the average row sum of $A_{i,j}$. Then the matrix B of order r with (i,j) entry equal to $b_{i,j}$ is called the *quotient matrix of A over $\{X_1, X_2, \ldots, X_r\}$*. If the row sum of each block $A_{i,j}$ is constant then the partition $\{X_1, X_2, \ldots, X_r\}$ is called *equitable (or regular)* and we have $A_{i,j}\mathbf{1}_{|X_j|} = b_{i,j}\mathbf{1}_{|X_j|}$, for each $1 \leq i, j \leq r$. Thus, $AS = SB$ and it follows that $B = K^{-1}S^TAS$. This gives rise to the following result, which says if λ is an eigenvalue of B then it is also an eigenvalue of A.

Theorem 1.5.1 *[8, 27] Let $\{X_1, X_2, \ldots, X_r\}$ be an equitable partition of A with characteristic matrix S. Let B be the quotient matrix of A over $\{X_1, X_2, \ldots, X_r\}$. If v is an eigenvector of B with corresponding eigenvalue λ, then Sv is an eigenvector of A with corresponding eigenvalue λ.*

An *equitable partition of a graph G* is an equitable partition of its adjacency matrix, that is, a partition of the vertex set V into parts $\{V_1, V_2, \ldots, V_r\}$ such that each vertex in V_i has the same number of neighbours in V_j, for any j. In particular, the number of neighbours that a vertex in V_i has in V_j is the (i,j)-entry of the quotient matrix B, namely $b_{i,j}$. An equivalent definition is that the subgraph of G induced by each part V_i is regular, and the edges joining any two distinct parts V_i and V_j form a semiregular bipartite graph. An *almost equitable partition of a graph* is a partition of the vertex set V into parts $\{V_1, V_2, \ldots, V_r\}$ such that each vertex in V_i has the same number of neighbours in V_j, for any $j \neq i$. In this case, the subgraph of G induced by each part V_i need not be regular, but the edges joining any two distinct parts V_i and V_j must form a semiregular bipartite graph.

Example 1.5.2 *We compute the ordinary spectrum of the complete bipartite graph $K_{p,q}$. Consider $K_{p,q}$ with parts X_1 and X_2, such that $|X_1| = p$ and $|X_2| = q$. Then the adjacency matrix can be partitioned as*

$$A = \begin{bmatrix} \mathbf{0}_{p\times p} & J_{p\times q} \\ J_{q\times p} & \mathbf{0}_{q\times q} \end{bmatrix}.$$

It is easy to see that 0 is an eigenvalue of A with multiplicity $p + q - 2$ by noting that the

vectors

$$\begin{bmatrix} 1 \\ -1 \\ 0 \\ \vdots \\ 0 \\ \hline \mathbf{0}_q \end{bmatrix}, \ldots, \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ -1 \\ \hline \mathbf{0}_q \end{bmatrix}, \begin{bmatrix} \mathbf{0}_p \\ \hline 1 \\ -1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} \mathbf{0}_p \\ \hline 1 \\ 0 \\ \vdots \\ 0 \\ -1 \end{bmatrix},$$

form a linearly independent set of $p+q-2$ null vectors for A. To find the two remaining eigenvalues we use the technique of equitable partitions.

Since each block of the partition of A has constant row sums, the partition $\{X_1, X_2\}$ is equitable. The quotient matrix B of A over $\{X_1, X_2\}$ is the 2×2 matrix

$$B = \begin{bmatrix} 0 & q \\ p & 0 \end{bmatrix},$$

whose entries are the (uniform) row sums of the blocks of A. The eigenvalues of B are $\pm\sqrt{pq}$, and thus these are also eigenvalues of A by Theorem 1.5.1.

1.6 Spectra of common classes of graphs

In this section we list the eigenvalues for some common classes of graphs with respect to the adjacency matrix, combinatorial Laplacian and the normalized Laplacian. We use the superscript notation $\lambda_i^{(m_i)}$ to mean that λ_i appears in the spectrum with multiplicity m_i.

Example 1.6.1 *The complete graph K_n. The ordinary spectrum is*

$$\{(-1)^{(n-1)},\ (n-1)^{(1)}\},$$

the combinatorial Laplacian spectrum is

$$\{0^{(1)},\ n^{(n-1)}\},$$

and the normalized Laplacian spectrum is

$$\left\{0^{(1)},\ \left(\frac{n}{n-1}\right)^{(n-1)}\right\}.$$

Example 1.6.2 *The complete bipartite graph $K_{p,q}$. As shown in Example 1.5.2, the ordinary spectrum is*

$$\{\pm\sqrt{pq}^{(1)},\ 0^{(p+q-2)}\}.$$

The combinatorial Laplacian spectrum is

$$\{0^{(1)},\ p^{(q-1)},\ q^{(p-1)},\ (p+q)^{(1)}\},$$

and the normalized Laplacian spectrum is

$$\left\{0^{(1)},\ 1^{(p+q-2)},\ 2^{(1)}\right\}.$$

Example 1.6.3 *The path P_n on n vertices. The ordinary spectrum is*

$$\left\{2\cos\left(\frac{\pi j}{n+1}\right) : j = 1, 2\ldots, n\right\},$$

the combinatorial Laplacian spectrum is

$$\left\{2-2\cos\left(\frac{\pi j}{n}\right) : j = 0, 1, \ldots, n-1\right\},$$

and the normalized Laplacian spectrum is

$$\left\{1-\cos\left(\frac{\pi j}{n-1}\right) : j = 0, 1, \ldots, n-1\right\}.$$

Example 1.6.4 *The cycle C_n on n vertices. The ordinary spectrum is*

$$\left\{2\cos\left(\frac{2\pi j}{n}\right) : j = 0, 1, \ldots, n-1\right\},$$

the combinatorial Laplacian spectrum is

$$\left\{2-2\cos\left(\frac{2\pi j}{n}\right) : j = 0, 1, \ldots, n-1\right\},$$

and the normalized Laplacian spectrum is

$$\left\{1-\cos\left(\frac{2\pi j}{n}\right) : j = 0, 1, \ldots, n-1\right\}.$$

Example 1.6.5 *The Petersen graph is a graph on 10 vertices depicted in Figure 1.10. The ordinary spectrum is*

$$\{(-2)^{(4)},\ 1^{(5)},\ 3^{(1)}\},$$

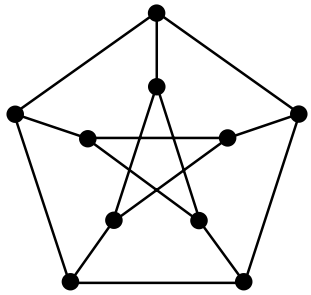

Figure 1.10: The Petersen graph.

the combinatorial Laplacian spectrum is

$$\{0^{(1)},\ 2^{(5)},\ 5^{(4)}\},$$

and the normalized Laplacian spectrum is

$$\left\{0^{(1)},\ \left(\frac{2}{3}\right)^{(5)},\ \left(\frac{5}{3}\right)^{(4)}\right\}.$$

Example 1.6.6 *Let G be a regular graph of degree r. Then we have the following relationship amongst A, L and $\mathcal{L}$:*

$$L = r\mathcal{L} = rI - A.$$

Thus, if the eigenvalues of one of A, L or $\mathcal{L}$ is known, the eigenvalues of the other two can be completely determined through the equation $\lambda(L) = r\lambda(\mathcal{L}) = r - \lambda(A)$.

To illustrate, we note that the Petersen graph in Example 1.6.5 is regular of degree 3. Thus, the L-spectrum and $\mathcal{L}$-spectrum can be obtained from the ordinary spectrum using $\lambda(L) = 3 - \lambda(A)$ and $\lambda(\mathcal{L}) = 1 - \frac{\lambda(A)}{3}$.

1.7 Energy of graphs and matrices

If G is a graph of order n and M is a real symmetric matrix associated with G, then the *M-energy* of G is

$$E_M(G) = \sum_{i=1}^{n} \left|\lambda_i(M) - \frac{tr(M)}{n}\right|. \tag{1.1}$$

The *energy* of a graph simply refers to using the adjacency matrix in (1.1). Gutman [29] introduced the energy of a graph in 1978 from a theoretical chemistry perspective. Recently,

the energy [30], Laplacian energy [32], signless Laplacian energy, distance energy [54] and incidence energy [31] of a graph have received much interest. Along the same lines, the energy of more general matrices and sequences has been studied (see [1, 50]). The goal of this thesis is to analyze the $\mathcal{L}$-energy of a graph, and determine how graph structure relates to $\mathcal{L}$-energy.

Throughout this thesis we will usually assume that the graphs encountered have no isolated vertices, since they contribute little information and add technicalities to the arguments. Thus, for a graph without isolated vertices, $tr(\mathcal{L}) = n$. Formally, using (1.1) with M taken to be $\mathcal{L}$, the *normalized Laplacian energy* (or *$\mathcal{L}$-energy*) of a graph G of order n is

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{n} |\lambda_i(\mathcal{L}) - 1|.$$

It is easy to see that this is equivalent to

$$\begin{aligned} E_{\mathcal{L}}(G) &= \sum_{i=1}^{n} |\lambda_i(I - \mathcal{L})|, && (1.2) \\ &= \sum_{i=1}^{n} \sigma_i(I - \mathcal{L}). && (1.3) \end{aligned}$$

Observe that Nikiforov [50] defines the energy of a matrix M of order n to be

$$\mathcal{E}(M) = \sum_{i=1}^{n} \sigma_i(M),$$

in which case by (1.3) we are interested in $\mathcal{E}(I - \mathcal{L})$. In this thesis we use the M-energy definition in (1.1) when referring to the energy of a real symmetric matrix.

1.8 Energy in terms of mean deviations

The energy of a matrix can be thought of as the deviation of its eigenvalues from the mean. In particular, given a data set $X = \{x_1, x_2, \ldots, x_n\}$ of real numbers, the *mean absolute deviation* (often called the *mean deviation*) is defined by

$$\mathrm{MD}(X) = \frac{1}{n} \sum_{i=1}^{n} |x_i - \bar{x}|,$$

where $\bar{x}$ is the arithmetic mean of the distribution. Often in statistical dispersion, the mean is replaced by the median in the above formula (or some other chosen measure of central

tendency of the data set). Statistical dispersion and central tendency are the most used properties of distributions. The focus of statistical dispersion is on measuring the spread in a variable or probability distribution while central tendency relates to the way in which data tend to cluster around some value. The mean deviation tells us the average amount that the data values deviate from the mean and is an intuitive and reasonable measure of dispersion. However, in practice, the average of the squared deviations from the mean, called the variance, is preferred. The *variance* of a data set $X = \{x_1, x_2, \ldots, x_n\}$, denoted by $\mathrm{Var}(X)$, is defined to be

$$\mathrm{Var}(X) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2.$$

The *standard deviation* is the square root of the variance. The mean deviation is an important descriptive statistic but the standard deviation is more frequently encountered in statistics. This is because the absolute value in mean deviation makes analytical calculations more complicated than using the standard deviation.

An easy application of the Cauchy-Schwarz inequality gives that the mean deviation is a lower bound on the standard deviation, in other words

$$\mathrm{MD}(X) \leq \sqrt{\mathrm{Var}(X)}.$$

Hence,

$$\sum_{i=1}^{n}|x_i - \bar{x}| \leq \sqrt{n\sum_{i=1}^{n}(x_i - \bar{x})^2}.$$

If M is a real symmetric matrix of order n associated with G, then

$$\begin{aligned} E_M(G) &= n \cdot \mathrm{MD}(\{\lambda_1(M), \lambda_2(M), \ldots, \lambda_n(M)\}) \\ &\leq \sqrt{n\sum_{i=1}^{n}\left(\lambda_i(M) - \frac{tr(M)}{n}\right)^2}. \end{aligned}$$

Many of the upper bounds for different types of energy stated in the literature are in fact instances of the bound above (for example, see [11, 32, 47, 54]).

1.9 The general Randić index of graphs

Let G be a graph of order n (with no isolated vertices). A well studied parameter of G is the *general Randić index* $R_\alpha(G)$, defined as

$$R_\alpha(G) = \sum_{x\sim y} (d_x d_y)^\alpha \,, \tag{1.4}$$

where the summation is over all (unordered) edges xy in G, and $\alpha \neq 0$ is a fixed real number. In 1975, Randić [55] proposed a topological index R (with $\alpha = -\frac{1}{2}$) under the name 'branching index'. In 1998, Bollobás and Erdős [4] generalized this index by replacing the $-1/2$ with any real number α (as defined in (1.4)). The papers [41, 42] survey recent results on the general Randić index of graphs with an emphasis on trees and chemical graphs. In Chapter 2 we will focus on the case when $\alpha = -1$ and show its importance to $\mathcal{L}$-energy and the spectrum of $\mathcal{L}$.

The general Randić index when $\alpha = -1$ is

$$R_{-1}(G) = \sum_{x\sim y} \frac{1}{d_x d_y}. \tag{1.5}$$

We now rewrite the above summation as a double summation using the following equation:

$$2\sum_{x\sim y} f(x,y) = \sum_{y\in V} \sum_{\substack{x \\ x\sim y}} f(x,y), \tag{1.6}$$

where

$$\sum_{\substack{x \\ x\sim y}} f(x,y)$$

represents the sum over all (unordered) edges xy in G that are incident to a fixed vertex y in the vertex set V of G. By rewriting (1.5) we obtain,

$$R_{-1}(G) = \frac{1}{2}\sum_{y\in V} \frac{1}{d_y} \sum_{\substack{x \\ x\sim y}} \frac{1}{d_x}. \tag{1.7}$$

Using (1.5), the quantity $R_{-1}(G)$ can be found by putting a weight of $\frac{1}{d_x d_y}$ on each edge xy of G (which we call the *weight of edge* xy), and then summing the weights over all the edges of G. Alternatively, using (1.7), $R_{-1}(G)$ can be found by putting a weight of

$$\frac{1}{2d_y} \sum_{\substack{x \\ x\sim y}} \frac{1}{d_x}$$

on each vertex y of G (which we call the *weight of vertex* y), and then summing the weights over all the vertices of G.

It is easy to compute $R_{-1}(G)$ for common classes of graphs by using an edge weighted graph as described above. We illustrate this below by computing $R_{-1}(G)$ for a path, complete bipartite graphs and regular graphs.

Example 1.9.1 *If G is a path on n vertices, then the leaf edges will have a weight of $\frac{1}{2}$ each and every other edge will have a weight of $\frac{1}{4}$ (see Figure 1.11).*

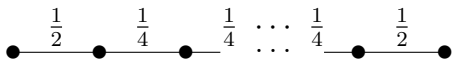

Figure 1.11: The (edge) weighted graph of a path corresponding to $R_{-1}(G)$.

Hence, $R_{-1}(G) = (n-3) \cdot \frac{1}{4} + 2 \cdot \frac{1}{2} = \frac{n+1}{4}$.

Example 1.9.2 *If G is a complete bipartite graph, $K_{p,q}$, then every edge will have weight $\frac{1}{pq}$. Since there are pq edges, we have that $R_{-1}(G) = 1$.*

Example 1.9.3 *If G is an r-regular graph of order n, then every edge will have weight $\frac{1}{r^2}$. Since there are $\frac{nr}{2}$ edges, we have that $R_{-1}(G) = \frac{n}{2r}$. In particular, the complete graph has $R_{-1}(G) = \frac{n}{2(n-1)}$. For n even, the graph G that is the disjoint union of $\frac{n}{2}$ paths of length 1 has $R_{-1}(G) = \frac{n}{2}$.*

2 EIGENVALUES OF THE NORMALIZED LAPLACIAN

2.1 Introduction

In the literature, the adjacency matrix and combinatorial Laplacian have been more widely used than the normalized Laplacian. One reason for this is because the normalized Laplacian is a rather new tool which has rather recently (mid 1990's) been popularized by Chung [12]. One of the original motivations for defining the normalized Laplacian was to be able to deal more naturally with non-regular graphs. In some situations the normalized Laplacian is a more natural tool that works better than the adjacency matrix or combinatorial Laplacian. In particular, when dealing with random walks, the normalized Laplacian is a natural choice, as demonstrated in Section 2.3. This is because $Q = D^{-1}A$ is the transition matrix of a Markov chain which has the same eigenvalues as $I - \mathcal{L}$. The spectrum of Q is studied in [17] and was the viewpoint of Runge's dissertation in 1976 (see [56]).

In this chapter, we focus on the spectrum of the normalized Laplacian matrix of a graph. We first list some basic properties of the spectrum and discuss the relationship between simple random walks on graphs and normalized Laplacian eigenvalues. We then discuss the importance of the largest eigenvalue of $\mathcal{L}$ and its relationship to bipartite graphs. Next we construct cospectral graphs with respect to the $\mathcal{L}$-eigenvalues by using Godsil-McKay switching. The graphs constructed answer two questions asked by Butler in [9]. We then look at properties of graphs with two or three distinct normalized Laplacian eigenvalues. The case that a graph has a vertex of degree 1 and exactly three distinct $\mathcal{L}$-eigenvalues is looked at. We next outline the important relationship that the general Randić index has with the spectrum of the normalized Laplacian. Finally, we rewrite some of the results developed by Runge in the 1970's in terms of the $\mathcal{L}$-eigenvalues. This includes a Matrix-Tree Theorem and Coefficients Theorem for $\mathcal{L}$.

2.2 Basic facts about the spectrum

Let G be a graph of order n. As $\mathcal{L}$ is a real symmetric matrix, the eigenvalues are real numbers. We note that normalized Laplacian $\mathcal{L}$ of G is a positive semidefinite matrix. To see this, let S be the matrix, whose rows are indexed by the vertices of G and whose columns are indexed by the edges of G (where each edge $e = xy$ is thought of as an ordered 2-tuple (x, y)), that has entries

$$S(u,e) = \begin{cases} \frac{1}{\sqrt{d_x}} & \text{if } e = xy \text{ and } u = x, \\ -\frac{1}{\sqrt{d_y}} & \text{if } e = xy \text{ and } u = y, \\ 0 & \text{otherwise.} \end{cases}$$

The choice of signs can actually be arbitrary so long as in each column (corresponding to an edge of G) there is one positive entry and one negative entry. Then $\mathcal{L} = SS^T$. Therefore, by Theorem 1.4.3, all of the eigenvalues of $\mathcal{L}$ are nonnegative.

Recall that D is the diagonal matrix of vertex degrees of a graph, namely,

$$D(u,v) = \begin{cases} d_u & \text{if } u = v, \\ 0 & \text{otherwise.} \end{cases}$$

It is easy to see that $D^{1/2}\mathbf{1}$ is an eigenvector of $\mathcal{L}$ with eigenvalue 0. Thus, we assume the eigenvalues of $\mathcal{L}$ are

$$0 = \lambda_1(\mathcal{L}) \leq \lambda_2(\mathcal{L}) \leq \cdots \leq \lambda_n(\mathcal{L}).$$

For graphs without isolated vertices, the normalized Laplacian $\mathcal{L}$ has the following relationship to L, A and D,

$$\begin{aligned} \mathcal{L} &= D^{-1/2}LD^{-1/2}, \\ &= D^{-1/2}(D-A)D^{-1/2}, \\ &= I - D^{-1/2}AD^{-1/2}. \end{aligned}$$

As mentioned in Example 1.6.6, if G is a regular graph then the eigenvalues of A, L and $\mathcal{L}$ are related by scaling factors and translations. However, for general graphs, the eigenvalues of A, L and $\mathcal{L}$ behave quite differently.

Using Sylvester's law of inertia (see Theorem 1.4.5), we can relate the eigenvalues of $\mathcal{L}$ and A. In particular,

$$i(I - \mathcal{L}) = i(D^{-1/2}AD^{-1/2}) = i(A).$$

Hence, the multiplicity of 0 as an eigenvalue for A equals the multiplicity of 1 as an eigenvalue for $\mathcal{L}$. Further, positive (resp. negative) eigenvalues of A correspond to eigenvalues in $[0, 1)$ (resp. $(1, \infty)$) for $\mathcal{L}$.

To get an idea of how the magnitudes of the eigenvalues between $\mathcal{L}$ and A (as well as $\mathcal{L}$ and L) relate, we use Theorem 1.4.6. Part (i) of the next theorem was first proved independently by Butler [10, Theorem 4] using the Courant-Fischer Theorem (see [36, Theorem 4.2.11]). We provide a new proof for part (i) and use this proof technique to obtain a relationship between the eigenvalues of $\mathcal{L}$ and A in part (ii).

Theorem 2.2.1 *Let G be a graph of order n with no isolated vertices. Suppose that G has minimum degree $d_{\min}$ and maximum degree $d_{\max}$. Let s be such that*

$$\lambda_1(A) \leq \cdots \leq \lambda_s(A) \leq 0 < \lambda_{s+1}(A) \leq \cdots \leq \lambda_n(A).$$

Then the following statements hold.

(i) [10, Theorem 4] For each $1 \leq k \leq n$,

$$\frac{\lambda_k(L)}{d_{\max}} \leq \lambda_k(\mathcal{L}) \leq \frac{\lambda_k(L)}{d_{\min}}.$$

(ii) For each $1 \leq k \leq n$,

$$\frac{|\lambda_{n-k+1}(A)|}{d_{\max}} \leq |1 - \lambda_k(\mathcal{L})| \leq \frac{|\lambda_{n-k+1}(A)|}{d_{\min}}.$$

In particular, for each $1 \leq k \leq n - s$,

$$1 - \frac{\lambda_{n-k+1}(A)}{d_{\min}} \leq \lambda_k(\mathcal{L}) \leq 1 - \frac{\lambda_{n-k+1}(A)}{d_{\max}},$$

and for each $n - s + 1 \leq k \leq n$,

$$1 - \frac{\lambda_{n-k+1}(A)}{d_{\max}} \leq \lambda_k(\mathcal{L}) \leq 1 - \frac{\lambda_{n-k+1}(A)}{d_{\min}}.$$

Proof. For (i), let M be the Laplacian matrix L and S be the matrix $D^{-1/2}$ in Theorem 1.4.6. As $D^{-1/2}$ is nonsingular, for each $k = 1, 2, \ldots, n$, there is a positive real number θ_k such that

$$\frac{1}{d_{\max}} = \lambda_1(D^{-1}) \leq \theta_k \leq \lambda_n(D^{-1}) = \frac{1}{d_{\min}}$$

and

$$\lambda_k(\mathcal{L}) = \theta_k \lambda_k(L).$$

Thus (i) now follows as the eigenvalues of both $\mathcal{L}$ and L are nonnegative.

For (ii), let M be the adjacency matrix A and S be the matrix $D^{-1/2}$ in Theorem 1.4.6. As $D^{-1/2}$ is nonsingular, for each $k = 1, 2, \ldots, n$, there is a positive real number θ_k such that

$$\frac{1}{d_{\max}} = \lambda_1(D^{-1}) \leq \theta_k \leq \lambda_n(D^{-1}) = \frac{1}{d_{\min}}$$

and

$$\lambda_k(I - \mathcal{L}) = \theta_k \lambda_k(A).$$

This is because $D^{-1/2} A D^{-1/2} = I - \mathcal{L}$. Using $\lambda_k(I - \mathcal{L}) = 1 - \lambda_{n-k+1}(\mathcal{L})$ and a relabeling of the indices gives,

$$1 - \lambda_k(\mathcal{L}) = \theta_{n-k+1} \lambda_{n-k+1}(A),$$

from which (ii) follows. □

A technique to obtain information about the eigenvalues of $\mathcal{L}$ relies on using the Rayleigh quotient (see [8] and [36, Theorem 4.2.2]). Below, we use the notation $\langle x_1, \ldots, x_m \rangle$ to represent the span of the vectors $\{x_1, \ldots, x_m\}$, and $\langle x_1, \ldots, x_m \rangle^{\perp}$ to represent the *orthogonal complement* of $\langle x_1, \ldots, x_m \rangle$, that is, the set of vectors y such that y is orthogonal to all vectors in $\langle x_1, \ldots, x_m \rangle$.

Let M be a real symmetric matrix of order n and $\{g_1, g_2, \ldots, g_n\}$ be an orthonormal set of eigenvectors of M corresponding to the eigenvalues

$$\{\lambda_1(M), \lambda_2(M), \ldots, \lambda_n(M)\},$$

that is, $M g_i = \lambda_i(M) g_i$, for each i. As M is a real symmetric matrix, the span of $\{g_1, g_2, \ldots, g_n\}$ is equal to $\mathbb{R}^n$. The Rayleigh Principle states that if $g \neq \mathbf{0}_n$, then

$$\lambda_i(M) \geq \frac{g^T M g}{g^T g}, \qquad \text{if } g \in \langle g_1, \ldots, g_{i-1} \rangle^{\perp},$$

and

$$\lambda_i(M) \leq \frac{g^T M g}{g^T g}, \qquad \text{if } g \in \langle g_1, \ldots, g_i \rangle.$$

In both cases, equality implies that g is an eigenvector of M with eigenvalue $\lambda_i(M)$.

Let $G = (V, E)$ be a graph. We can view the eigenvectors g of $\mathcal{L}$ as functions which assign to each vertex v of G a real value $g(v)$. In particular, if $V = \{v_1, v_2, \ldots, v_n\}$ and

$g = [\gamma_1, \gamma_2, \ldots, \gamma_n]^T$, then g can be viewed as a function which assigns to each vertex v_i the real value γ_i, that is, $g(v_i) = \gamma_i$. By letting $g = D^{1/2}f$, we have

$$\begin{aligned}\frac{g^T\mathcal{L}g}{g^Tg} &= \frac{f^TD^{1/2}\mathcal{L}D^{1/2}f}{(D^{1/2}f)^TD^{1/2}f},\\ &= \frac{f^TLf}{f^TDf},\\ &= \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v f(v)^2d_v}.\end{aligned}$$

Thus, we obtain the following formulas for $\lambda_2(\mathcal{L})$ and $\lambda_n(\mathcal{L})$ (see [12] for more detail):

$$\lambda_2(\mathcal{L}) = \inf_{f\perp D\mathbf{1}} \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v f(v)^2d_v}, \tag{2.8}$$

$$\lambda_n(\mathcal{L}) = \sup_{f\neq 0} \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v f(v)^2d_v}. \tag{2.9}$$

A vector f that satisfies equality in (2.8) or (2.9) is called a *harmonic eigenfunction* of $\mathcal{L}$. If f satisfies (2.8) with equality then

$$\mathcal{L}\left(D^{1/2}f\right) = \lambda_2(\mathcal{L})\left(D^{1/2}f\right),$$

that is, $D^{1/2}f$ is an eigenvector of $\mathcal{L}$ with eigenvalue $\lambda_2(\mathcal{L})$. Similarly, if f satisfies (2.9) with equality then $D^{1/2}f$ is an eigenvector of $\mathcal{L}$ with eigenvalue $\lambda_n(\mathcal{L})$.

The next lemma lists several basic properties about the normalized Laplacian eigenvalues, all of which can be found in [12].

Lemma 2.2.2 *[12] Let G be a graph of order $n \geq 2$ that contains no isolated vertices.*

(1) $\sum_{i=1}^{n}\lambda_i(\mathcal{L}) = n.$

(2) $\lambda_2(\mathcal{L}) \leq \frac{n}{n-1}$ *with equality holding if and only if G is the complete graph on n vertices.*

(3) $\lambda_n(\mathcal{L}) \geq \frac{n}{n-1}$ *with equality holding if and only if G is the complete graph on n vertices.*

(4) If G is not the complete graph then $\lambda_2(\mathcal{L}) \leq 1$.

(5) If G is connected with m edges and diameter D, then $\lambda_2(\mathcal{L}) \geq \frac{1}{2mD} > 0$.

(6) If $\lambda_i(\mathcal{L}) = 0$ and $\lambda_{i+1}(\mathcal{L}) \neq 0$, then G has exactly i connected components (that is, the number of connected components of G is equal to the multiplicity of the eigenvalue 0).

(7) For each $1 \leq i \leq n$, we have $\lambda_i(\mathcal{L}) \in [0, 2]$.

(8) The $\mathcal{L}$-spectrum of a graph is the union of $\mathcal{L}$-spectra of its connected components.

(9) $\lambda_n(\mathcal{L}) = 2$ if and only if a connected component of G is bipartite.

(10) G is bipartite if and only if the number of connected components equals the multiplicity of the eigenvalue 2.

(11) G is bipartite if and only if for each $\lambda_i(\mathcal{L})$, the value $2 - \lambda_i(\mathcal{L})$ is also an eigenvalue of G.

Proof. We illustrate some parts of the proof to demonstrate how (2.8) and (2.9) can be used.

(1) This follows from $tr(\mathcal{L}) = n$.

The inequalities in (2) and (3) follow from

$$\sum_{i=2}^{n} \lambda_i(\mathcal{L}) = n,$$

which implies that the average of $\{\lambda_2(\mathcal{L}), \ldots, \lambda_n(\mathcal{L})\}$ is $\frac{n}{n-1}$.

(4) This can be illustrated by considering two nonadjacent vertices x, y, and using $\hat{f}$ defined as

$$\hat{f}(v) = \begin{cases} d_y & \text{if } v = x, \\ -d_x & \text{if } v = y, \\ 0 & \text{otherwise,} \end{cases}$$

along with (2.8).

(7) The upper bound of 2 uses (1.6) and (2.9), and the fact that

$$[f(u) - f(v)]^2 \leq 2f^2(u) + 2f^2(v).$$

(11) To see why the normalized Laplacian eigenvalues of a bipartite graph are symmetric about 1 (including multiplicities), note that $I - \mathcal{L}$ can be written as

$$\begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix} = \begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & -B \\ -B^T & 0 \end{bmatrix} \begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix}.$$

Thus, $(I - \mathcal{L})$ and $-(I - \mathcal{L})$ have the same spectrum for bipartite graphs. □

The largest normalized Laplacian eigenvalue $\lambda_n(\mathcal{L})$ tells us when a graph is bipartite. In Section 2.4 we will look at $\lambda_n(\mathcal{L})$ in more detail.

2.3 Relationship to random walks on graphs

In this section we investigate how the normalized Laplacian spectrum of a graph can provide information about random walks on graphs. Applications of random walks on graphs range from sampling problems, electrical networks, routing problems, queuing theory, and even shuffling a deck of cards. For a survey paper about random walks on graphs see [46]. For more details regarding the relationship of random walks on graphs to the normalized Laplacian see [10, 12]. It should be pointed out that as early as 1935, Bottema considered the relationship between $D^{-1}A$ and random walks in a connected graph [5, 17]. All of the details from this section are known results that come from [10, 12, 40, 46] and are meant to illustrate the importance of the eigenvalues of $\mathcal{L}$.

A *random walk on a graph* can be thought of as a walk where we start at a vertex in the graph and at each time interval randomly pick an edge incident to the current vertex to traverse, and repeat. It turns out that random walks on (simple, undirected) graphs are examples of Markov chains. We first describe some terminology from stochastic processes that will be used in this section which can be found in [40].

A *discrete-time stochastic process* is a random process evolving with discrete time. Specifically, it is a collection of random variables $\{X_1, X_2, X_3, \ldots\}$ indexed by time, where time is a subset of $\{1, 2, 3, \ldots\}$, and X_i takes values in the finite set $S = \{1, 2, \ldots, n\}$. The possible values for X_i are called the *states* of the system. A *Markov chain* is a discrete-time stochastic process with the *Markov property*, namely that, given the present state (corresponding to time t), the future state (at time $t + 1$) and past states (at times before t) are independent:

$$\Pr(X_{t+1} = i_{t+1} | X_1 = i_1, \ldots, X_t = i_t) = \Pr(X_{t+1} = i_{t+1} | X_t = i_t),$$

where $\Pr(A)$ represents the probability of event A. To describe the probabilities for such a process we give the initial probability distribution

$$f(i) = \Pr(X_1 = i), \qquad i = 1, 2, \ldots, n,$$

and the *transition probabilities*

$$\Pr(X_{t+1} = i_{t+1} | X_t = i_t).$$

We will be dealing with *time-homogeneous* Markov chains where the transition probabilities do not depend on time. That is,

$$\Pr(X_{t+1} = i_{t+1} | X_t = i_t) = p(i_t, i_{t+1}),$$

for some function $p : S \times S \to [0, 1]$. The *transition matrix* P for a Markov chain is the matrix of order n whose (i, j)-entry is $p(i, j)$. We say P is *irreducible* if for any $i, j \in S$, there exists some k such that $P^k(i, j) > 0$. If P is the transition matrix for an irreducible Markov chain, we define the *period* of state i to be the greatest common divisor of $\{k \geq 0 : P^k(i, j) > 0\}$. It is easy to show that all states have the same period, thus we can talk about the period of P. If the period of P is one, then we call P *aperiodic*.

Let $G = (V, E)$ be a graph with adjacency matrix A and matrix of degrees D. Consider a Markov chain whose states are vertices in V. At each time interval, the chain chooses a new state randomly from among the states adjacent to the current state. The transition matrix for this chain is $P = D^{-1}A$, whose (i, j)-entry gives the probability that a move is made from vertex i to vertex j, in particular,

$$P(i, j) = (D^{-1}A)(i, j) = \begin{cases} \dfrac{1}{d_i} & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

A random walk is determined by the transition probabilities

$$P(i, j) = \Pr(X_{t+1} = j | X_t = i),$$

which are independent of t.

Let the vector f be an initial probability distribution. It is easy to see that the probability distribution after k steps is $f^T P^k$. To see the connection with $\mathcal{L}$, we note that the transition matrix is similar to $I - \mathcal{L}$ through the equation:

$$P = D^{-1}A = D^{-1/2}(I - \mathcal{L})D^{1/2}.$$

Thus, if λ is an eigenvalue of $\mathcal{L}$, then $1 - \lambda$ is an eigenvalue of P. In particular, 1 is always an eigenvalue of P as 0 is always an eigenvalue of $\mathcal{L}$.

A random walk in a graph is said to be *ergodic* if there is a unique *stationary distribution* π such that

$$\lim_{k \to \infty} f^T (D^{-1}A)^k = \pi.$$

It is well known that necessary and sufficient conditions for the ergodicity of P are irreducibility and aperiodicity of P.

A problem of interest is given any arbitrary initial distribution, determine the number of steps k required for P^k to be close to its stationary distribution. The transition matrix P satisfies

$$\mathbf{1}_n^T DP = \mathbf{1}_n^T D.$$

Therefore, the stationary distribution is

$$\pi = \frac{\mathbf{1}_n^T D}{\sum_{i=1}^n d_i}.$$

We ask if for any initial distribution f, does $f^T P^k$ converge to the stationary distribution? We consider the convergence in the L^2-norm (Euclidean norm). Note that different types of measurements will give different bounds for the rate of convergence. Some other bounds can be found in [12]. Let f be any initial probability distribution (so that $f^T \mathbf{1}_n = 1$). As shown in [10, 12], the Euclidean distance between the random walk after k steps and the stationary distribution π is

$$||f^T P^k - \pi|| \quad \leq \quad \max_{i \neq 1} |1 - \lambda_i(\mathcal{L})|^k \frac{\max_i \sqrt{d_i}}{\min_i \sqrt{d_i}}.$$

Thus, the $\mathcal{L}$-eigenvalues can be used to get an estimate on the rate of convergence of a random walk. In particular, the closer the $\mathcal{L}$-eigenvalues (omitting 0) are gathered around 1, the faster we expect to converge to the stationary distribution. In turn, this provides an estimate on the number of steps needed to produce random-like results.

It should be noted that as $\lambda_i(\mathcal{L}) \in [0, 2]$, we have

$$\max_{i \neq 1} |1 - \lambda_i(\mathcal{L})| \leq 1.$$

As seen in Lemma 2.2.2, there are two ways $\max_{i \neq 1} |1 - \lambda_i(\mathcal{L})|$ can equal 1. The first is if $\lambda_2(\mathcal{L}) = 0$, which implies the graph G is not connected. The second is if $\lambda_n = 2$, which implies the graph has a bipartite component. Therefore, for a random walk to converge to the stationary distribution it suffices to be on a graph that is connected and not bipartite. A graph being connected is equivalent to the system being irreducible, and a graph being non-bipartite is equivalent to the system being aperiodic. If $\max_{i \neq 1} |1 - \lambda_i(\mathcal{L})| < 1$, then we have the existence and uniqueness of a stationary distribution as our random walk is ergodic.

2.4 Discussion on the largest normalized Laplacian eigenvalue

In this section we will focus on (2.9) to obtain information about $\lambda_n(\mathcal{L})$. By Lemma 2.2.2 we have the following bounds on $\lambda_n(\mathcal{L})$:

$$\frac{n}{n-1} \leq \lambda_n(\mathcal{L}) \leq 2,$$

with equality in the lower bound if and only if G is the complete graph and equality in the upper bound if and only if G contains a bipartite component. In what follows we show an intuitive interpretation of $\lambda_n(\mathcal{L})$. In particular, we show that the "closer" a graph is to being bipartite, the closer $\lambda_n(\mathcal{L})$ is to 2. It should be noted that a similar statement for r-regular graphs and $\lambda_1(\frac{1}{r}A)$ is quantified by Trevisan [64] by introducing the concept of the bipartiteness ratio of a graph.

Let $G = (V, E)$ be a graph and let $S \subseteq V$ be a subset of the vertices. We denote the *complement* of the set S by $\bar{S}$, which is defined as $\bar{S} = V \backslash S$. The *volume* of S is a quantity that shows up a lot when dealing with the normalized Laplacian, and is defined to be the sum of the degrees of the vertices in S, that is,

$$\mathrm{vol}(S) = \sum_{x \in S} d_x.$$

Note that $\mathrm{vol}(V)$ is equal to twice the number of edges in the graph and is often denoted by $\mathrm{vol}(G)$. Given two subsets X, Y of the vertices of G, we define

$$e(X, Y) = |\{xy \in E : x \in X, y \in Y\}|,$$

with the convention that edges in $X \cap Y$ are counted twice.

The following result provides a bound on $\lambda_2(\mathcal{L})$ and $\lambda_n(\mathcal{L})$ based on a partition of the vertex set of the graph into two disjoint subsets.

Lemma 2.4.1 *Let G be a graph of order n. Then*

$$0 = \lambda_1(\mathcal{L}) \leq \lambda_2(\mathcal{L}) \leq \min_{\emptyset \neq S \subset V} \left(\frac{e(S, \bar{S})}{\mathrm{vol}(S)} + \frac{e(S, \bar{S})}{\mathrm{vol}(\bar{S})} \right)$$

$$\leq \max_{\emptyset \neq S \subset V} \left(\frac{e(S, \bar{S})}{\mathrm{vol}(S)} + \frac{e(S, \bar{S})}{\mathrm{vol}(\bar{S})} \right) \leq \lambda_n(\mathcal{L}).$$

Proof. Let $\emptyset \neq S \subset V$ and define f as follows,

$$f(u) = \begin{cases} \alpha & \text{if } u \in S, \\ \beta & \text{if } u \notin S. \end{cases}$$

We have,

$$\frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v f(v)^2 d_v} = \frac{(\alpha-\beta)^2 e(S,\bar{S})}{\alpha^2\sum_{x\in S} d_x + \beta^2 \sum_{x\in\bar{S}} d_x} = \frac{(\alpha-\beta)^2 e(S,\bar{S})}{\alpha^2 \mathrm{vol}(S) + \beta^2 \mathrm{vol}(\bar{S})}.$$

Choosing $\alpha = -\mathrm{vol}(\bar{S})$ and $\beta = \mathrm{vol}(S)$ gives

$$\frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v f(v)^2 d_v} = e(S,\bar{S})\left(\frac{1}{\mathrm{vol}(S)} + \frac{1}{\mathrm{vol}(\bar{S})}\right).$$

Note that with the choice of f, α and β above, we have $(D\mathbf{1})^T f = 0$. Then by (2.8) and (2.9) we are done. □

The upper bound on $\lambda_2(\mathcal{L})$ in Lemma 2.4.1 is related to isoperimetric problems. In particular, when dealing with isoperimetric problems the following question is of importance.

Question 2.4.2 *For a fixed number m, find a subset S with $m \leq \mathrm{vol}(S) \leq \mathrm{vol}(\bar{S})$ such that $e(S,\bar{S})$ is as small as possible.*

Cheeger constants are meant to answer this type of question. For $S \subset V$, define

$$h_G(S) = \frac{e(S,\bar{S})}{\min\{\mathrm{vol}(S), \mathrm{vol}(\bar{S})\}}.$$

The *Cheeger constant* h_G of a graph G is defined as

$$h_G = \min_S h_G(S).$$

Then it is clear that

$$\lambda_2(\mathcal{L}) \leq \min_{\emptyset\neq S\subset V}\left(\frac{e(S,\bar{S})}{\mathrm{vol}(S)} + \frac{e(S,\bar{S})}{\mathrm{vol}(\bar{S})}\right) \leq 2h_G.$$

The Cheeger constant is a well studied parameter and has been further related to $\lambda_2(\mathcal{L})$. In particular, if G is a connected graph, $\lambda_2(\mathcal{L}) \geq \frac{h_G^2}{2}$ (see [12, Theorem 2.2]). By taking the

minimum of $\text{vol}(S)$ and $\text{vol}(\bar{S})$ in the definition of the Cheeger constant, it seems that some important information may be lost. We illustrate this by analyzing the bound on $\lambda_n(\mathcal{L})$ and keeping both $\text{vol}(S)$ and $\text{vol}(\bar{S})$ in our discussion.

Fix a graph $G = (V, E)$ and let $S \subseteq V$. Let a_1 represent the number of edges with both endpoints in S, a_2 represent the number of edges with both endpoints in $\bar{S}$ and $b = e(S, \bar{S})$. Then the lower bound on $\lambda_n(\mathcal{L})$ in Lemma 2.4.1 can be written as

$$\lambda_n(\mathcal{L}) \geq \left(\frac{b}{2a_1 + b} + \frac{b}{2a_2 + b} \right).$$

If the graph is bipartite, S can be chosen so that $a_1 = a_2 = 0$, giving $\lambda_n(\mathcal{L}) \geq 2$. Increasing the number of edges between S and $\bar{S}$ (i.e., increasing b), or decreasing the number of edges with both ends in S or both ends in $\bar{S}$ (i.e., decreasing a_1 or a_2), have the effect of increasing the lower bound on $\lambda_n(\mathcal{L})$. It is in this sense that the closer a graph is to being bipartite (i.e., the more b edges or less a_1, a_2 edges there are), the closer $\lambda_n(\mathcal{L})$ is to 2.

Lemma 2.4.1 is a special case of a modified version of [10, Theorem 36] and should also be compared to [67, Lemma 4.28] where a lower bound on $\lambda_n(\mathcal{L})$ is given in terms of the size of the maximum cut of a graph. We note that Theorem 36 in [10] can be slightly improved by noticing that the matrix B in the proof is singular, and hence, λ_{n-m} in the far right summation can be excluded (as $\eta_1 = 0$ can be ignored). We rewrite the Theorem (in terms of our labeling of the eigenvalues) with the improvement of changing the $m - 1$ limit in the far right summation to $m - 2$.

Theorem 2.4.3 *[10, Theorem 36] Let G be a graph of order n with no isolated vertices. For every partitioning of the vertices $[n] = N_1 \cup \cdots \cup N_m$ we have*

$$\sum_{i=1}^{m} \lambda_i(\mathcal{L}) \leq m - \sum_{i=1}^{m} \frac{e(N_i, N_i)}{\text{vol}(N_i)} = \sum_{1 \leq i < j \leq m} e(N_i, N_j) \left(\frac{1}{\text{vol}(N_i)} + \frac{1}{\text{vol}(N_j)} \right) \leq \sum_{i=0}^{m-2} \lambda_{n-i}.$$

Based on Lemma 2.4.1, we ask the question:

Question 2.4.4 *For which graphs G does equality hold in*

$$\lambda_n(\mathcal{L}) \geq \max_{\emptyset \neq S \subset V} \left(\frac{e(S, \bar{S})}{\text{vol}(S)} + \frac{e(S, \bar{S})}{\text{vol}(\bar{S})} \right)?$$

In fact, for many graphs such as bipartite graphs, the complete graph, and the petal graph (see [12, Example 1.12] or Example 2.6.7 with $m = 2$), the bound on $\lambda_n(\mathcal{L})$ in Question 2.4.4 holds with equality. A partial answer to Question 2.4.4 is the following result.

Lemma 2.4.5 *Let $G = (V, E)$ be a graph of order n such that there is a partition $V = S \cup \bar{S}$ with $S, \bar{S} \neq \emptyset$ such that*

$$\lambda_n(\mathcal{L}) = \frac{e(S, \bar{S})}{\mathrm{vol}(S)} + \frac{e(S, \bar{S})}{\mathrm{vol}(\bar{S})}.$$

Then the following regularity conditions hold:
For each vertex $u \in S$,

$$\frac{e(u, \bar{S})}{\mathrm{vol}(u)} = \frac{e(S, \bar{S})}{\mathrm{vol}(S)}, \tag{2.10}$$

and for each vertex $u \in \bar{S}$,

$$\frac{e(u, S)}{\mathrm{vol}(u)} = \frac{e(S, \bar{S})}{\mathrm{vol}(\bar{S})}. \tag{2.11}$$

In the above, it is understood that $\mathrm{vol}(u) = d_u$ and $e(u, X)$ is the number of edges incident to u of the form ux with $x \in X$.

Proof. Suppose that equality holds for the eigenvalue $\mu = \lambda_n(\mathcal{L})$ and some partition $V = S \cup \bar{S}$ with $S, \bar{S} \neq \emptyset$, that is,

$$\mu = \frac{e(S, \bar{S})}{\mathrm{vol}(S)} + \frac{e(S, \bar{S})}{\mathrm{vol}(\bar{S})}.$$

Let the adjacency matrix of G follow the same partition as the vertices, that is

$$\begin{bmatrix} A & B \\ B^T & C \end{bmatrix},$$

where the columns of A are indexed by elements in S and the columns of C are indexed by elements in $\bar{S}$. Similarly, let the matrix of degrees follow the same partition, that is

$$\begin{bmatrix} D_A & 0 \\ 0 & D_C \end{bmatrix}.$$

For convenience, we let $\alpha = \mathrm{vol}(\bar{S})$ and $\beta = -\mathrm{vol}(S)$. Then

$$\mu = \frac{e(S, \bar{S})}{\alpha} - \frac{e(S, \bar{S})}{\beta}.$$

Since

$$f(u) = \begin{cases} \alpha & \text{if } u \in S, \\ \beta & \text{if } u \in \bar{S}, \end{cases}$$

satisfies (2.9) with equality, it must be that $g = D^{1/2}f$ is an eigenvector of $\mathcal{L}$ with the eigenvalue μ. We can write g as

$$g = \begin{bmatrix} \alpha D_A^{1/2}\mathbf{1} \\ \beta D_C^{1/2}\mathbf{1} \end{bmatrix},$$

where the all ones vector $\mathbf{1}$ is assumed to have the appropriate size in each spot it is used. The normalized Laplacian is

$$\mathcal{L} = \begin{bmatrix} I - D_A^{-1/2}AD_A^{-1/2} & -D_A^{-1/2}BD_C^{-1/2} \\ -D_C^{-1/2}B^TD_A^{-1/2} & I - D_C^{-1/2}CD_C^{-1/2} \end{bmatrix}.$$

Since g is an eigenvector for $\mathcal{L}$, we have

$$\mathcal{L}g = \begin{bmatrix} (\alpha D_A^{-1/2})(D_A\mathbf{1} - A\mathbf{1} - (\beta/\alpha)B\mathbf{1}) \\ (\beta D_C^{-1/2})(-(\alpha/\beta)B^T\mathbf{1} + D_C\mathbf{1} - C\mathbf{1}) \end{bmatrix} = \mu g.$$

Let $u \in V$ and write $d_u = \hat{d}_u + \bar{d}_u$, where $\bar{d}_u$ is the number of edges incident to u that have one endpoint in S and one endpoint in $\bar{S}$, and $\hat{d}_u$ is the number of edges incident to u with both endpoints in S or both endpoints in $\bar{S}$. We can extend this notion in the obvious way to

$$D_A = \hat{D}_A + \bar{D}_A \quad \text{and} \quad D_C = \hat{D}_C + \bar{D}_C.$$

We have

$$B\mathbf{1} = \bar{D}_A\mathbf{1}, \qquad B^T\mathbf{1} = \bar{D}_C\mathbf{1}, \qquad A\mathbf{1} = \hat{D}_A\mathbf{1}, \qquad C\mathbf{1} = \hat{D}_C\mathbf{1}.$$

Then,

$$\mathcal{L}g = \begin{bmatrix} \alpha D_A^{-1/2}(D_A - \hat{D}_A - (\beta/\alpha)\bar{D}_A)\mathbf{1} \\ \beta D_C^{-1/2}(-(\alpha/\beta)\bar{D}_C + D_C - \hat{D}_C)\mathbf{1} \end{bmatrix} = \begin{bmatrix} (1-\beta/\alpha)\bar{D}_A D_A^{-1}(\alpha D_A^{1/2}\mathbf{1}) \\ (1-\alpha/\beta)\bar{D}_C D_C^{-1}(\beta D_C^{1/2}\mathbf{1}) \end{bmatrix} = \mu g.$$

Hence, for each vertex $u \in S$,

$$\left(1 - \frac{\beta}{\alpha}\right)\frac{\bar{d}_u}{d_u} = \mu,$$

and for each vertex $u \in \bar{S}$,

$$\left(1 - \frac{\alpha}{\beta}\right)\frac{\bar{d}_u}{d_u} = \mu.$$

Thus, for each vertex $u \in S$,

$$\frac{\bar{d}_u}{d_u} = \frac{e(S,\bar{S})}{\mathrm{vol}(S)},$$

and for each vertex $u \in \bar{S}$,

$$\frac{\bar{d}_u}{d_u} = \frac{e(S, \bar{S})}{\text{vol}(\bar{S})}.$$

Hence, we require the regularity conditions (2.10) and (2.11) to be satisfied for the partition $V = S \cup \bar{S}$. □

It should be noted that the converse of Lemma 2.4.5 does not hold. If the regularity conditions (2.10) and (2.11) are satisfied for some partition $V = S \cup \bar{S}$, then μ (as defined in the proof) is guaranteed to be an eigenvalue of $\mathcal{L}$ since the vector g (as defined in the proof) will be a corresponding eigenvector. However, this does not guarantee that μ will be the largest eigenvalue.

Remark 2.4.6 *Let $G = (V, E)$ be a graph of order n such that the regularity conditions (2.10) and (2.11) are satisfied for some partition $V = S \cup \bar{S}$, with $S, \bar{S} \neq \emptyset$. Then*

$$\mu = \frac{e(S, \bar{S})}{\text{vol}(S)} + \frac{e(S, \bar{S})}{\text{vol}(\bar{S})}$$

is an $\mathcal{L}$-eigenvalue of G.

We illustrate with an example to show that μ in Remark 2.4.6 may not always be the largest normalized Laplacian eigenvalue.

Example 2.4.7 *Let G be the graph in Figure 2.1. The partition $V = S \cup \bar{S}$ in the figure satisfies the regularity conditions (2.10) and (2.11), thus, $\mu = 1 + \frac{1}{2} = \frac{3}{2}$ is an $\mathcal{L}$-eigenvalue of G. The $\mathcal{L}$-eigenvalues of G (rounded to 3 decimal places where necessary) are*

$$\{0,\ 0.196,\ 0.887,\ 1.5,\ 1.5,\ 1.917\}.$$

It is easy to see that there is no partition of V into two sets that satisfy the regularity conditions (2.10) and (2.11) and gives equality in the bound in Question 2.4.4.

One way to construct graphs that satisfy the regularity conditions (2.10) and (2.11) in Lemma 2.4.5 is to take the join of two regular graphs. In particular, we show that if G_1 is an r-regular graph on n vertices, G_2 is an s-regular graph on m vertices, with $r \leq m/2$ and $s \leq n/2$, then $G_1 \vee G_2$ satisfies Question 2.4.4 with equality.

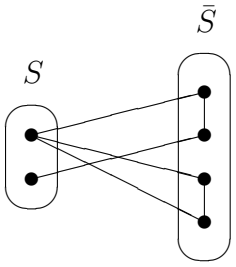

Figure 2.1: A graph satisfying the regularity conditions for a particular partition.

Example 2.4.8 *(Join of regular graphs) Let $G_1 = (V_1, E_1)$ be an r-regular graph on n vertices and $G_2 = (V_2, E_2)$ be an s-regular graph on m vertices. Suppose*

$$0 = \lambda_1 \leq \cdots \leq \lambda_n \leq 2$$

are the $\mathcal{L}$-eigenvalues of G_1 and

$$0 = \mu_1 \leq \cdots \leq \mu_n \leq 2$$

are the $\mathcal{L}$-eigenvalues of G_2. Butler [10, Theorem 12] proved that the $\mathcal{L}$-eigenvalues of $G_1 \vee G_2$ are

$$0, \frac{m + r\lambda_2}{m + r}, \ldots, \frac{m + r\lambda_n}{m + r}, \frac{n + s\mu_2}{n + s}, \ldots, \frac{n + s\mu_m}{n + s}, \frac{m}{m + r} + \frac{n}{n + s}.$$

If $r \leq m/2$ and $s \leq n/2$, then

$$\frac{m}{m + r} + \frac{n}{n + s} \geq \frac{2}{3} + \frac{2}{3} = \frac{4}{3}.$$

For each λ_i with $i \neq 1$,

$$\frac{m + r\lambda_i}{m + r} \leq \frac{m + 2r}{m + r} \leq \frac{4}{3}.$$

For each μ_i with $i \neq 1$,

$$\frac{n + s\mu_i}{n + s} \leq \frac{n + 2s}{n + s} \leq \frac{4}{3}.$$

Thus, when $r \leq m/2$ and $s \leq n/2$, $\frac{m}{m+r} + \frac{n}{n+s}$ is the largest normalized Laplacian eigenvalue of $G_1 \vee G_2$. In this case, $G_1 \vee G_2$ satisfies Question 2.4.4 with equality using the vertex partition $S = V_1$ and $\bar{S} = V_2$.

Finally, we remark that the two classes of graphs introduced in Section 2.6 in Examples 2.6.7 and 2.6.8 also satisfy Question 2.4.4 with equality.

2.5 Cospectral graphs with respect to the normalized Laplacian

Here we look at pairs of nonisomorphic graphs that have the same M-spectrum, where M is either A, L, $|L|$ or $\mathcal{L}$, although the results also hold for other matrix representations. Let G_1 and G_2 be r-regular graphs of the same order. If G_1 and G_2 are cospectral with respect to the A-eigenvalues, then they are also cospectral with respect to the L, $|L|$ and $\mathcal{L}$-eigenvalues by Example 1.6.6 and noting that $|L| = rI + A$. In [9, Theorem 2.1], Butler provides a construction of two nonisomorphic non-regular bipartite graphs which are cospectral with respect to both the adjacency and normalized Laplacian eigenvalues by reflecting a base bipartite graph in two different ways. However, the pairs of graphs that Butler constructs are not cospectral with respect to the combinatorial Laplacian eigenvalues. He then asks:

- Is there an example of two non-regular graphs which are cospectral with respect to the adjacency matrix, combinatorial Laplacian and normalized Laplacian at the same time?

- Are there general constructions which can be used to make cospectral graphs with respect to the normalized Laplacian which have arbitrarily high chromatic number?

Upon a discussion with S. Cioabă and W. Haemers *[personal communication, February 3rd, 2010]*, Haemers noted that non-regular graphs that are cospectral with respect to $\mathcal{L}$ (as well as A, L, and $|L|$) can be constructed using a technique due to Godsil and McKay. We describe this technique in detail which is then used to answer the two questions stated above.

In [26], Godsil and McKay consider a kind of switching operation on the edges of a graph and give conditions under which the adjacency spectrum is unchanged by this operation. We refer to their method as GM switching. This method of construction produces 72% of the cospectral graphs on nine vertices with respect to the A-eigenvalues [16], and has been applied to other matrix representations. For example, see [20, 21] where the authors survey the cases for which the answer to the question *"which graphs are determined by their spectrum"* is known for various matrix representations of graphs.

In the following new result, we show how GM switching can work for $\mathcal{L}$. Note that the next result is a special case of [33, Theorem 2] (which in turn, is a special case of the results in [26]). For notational purposes, we use the convention that $J_{s\times 0}$ and $J_{0\times s}$ (resp. $\mathbf{0}_{s\times 0}$ and

$\mathbf{0}_{0\times s}$) do not appear in the matrices A and $\hat{A}$ in Theorem 2.5.1 below in the case that $t_2 = 0$ (resp. $t_3 = 0$).

Theorem 2.5.1 *Let A and $\hat{A}$ be the following matrices of order $n = s + t$:*

$$A = \left[\begin{array}{c|ccc} A_{1,1} & N & J_{s\times t_2} & \mathbf{0}_{s\times t_3} \\ \hline N^T & & & \\ J_{t_2\times s} & & A_{2,2} & \\ \mathbf{0}_{t_3\times s} & & & \end{array}\right]$$

and

$$\hat{A} = \left[\begin{array}{c|ccc} A_{1,1} & (J_{s\times t_1} - N) & J_{s\times t_2} & \mathbf{0}_{s\times t_3} \\ \hline (J_{s\times t_1} - N)^T & & & \\ J_{t_2\times s} & & A_{2,2} & \\ \mathbf{0}_{t_3\times s} & & & \end{array}\right],$$

where N is a $(0,1)$-matrix of size $s \times t_1$, $A_{1,1}$ is a real symmetric matrix of order s, and $A_{2,2}$ is a real symmetric matrix of order t, where $t = t_1 + t_2 + t_3$, for $s \geq 4$ even, $t_1 \geq 2$ even and $t_2, t_3 \geq 0$. Suppose for some r that

$$A_{1,1}\mathbf{1}_s = r\mathbf{1}_s, \quad N\mathbf{1}_{t_1} = \frac{t_1}{2}\mathbf{1}_s, \quad \textit{and} \quad N^T\mathbf{1}_s = \frac{s}{2}\mathbf{1}_{t_1}.$$

Then the matrices A and $\hat{A}$ have the same spectrum.

Further, let D be a diagonal matrix of order n with diagonal entries $D(i,i)$ equal the sum of the entries in the ith row of A, for $1 \leq i \leq n$. Let M be a linear combination of products of nonnegative integer powers of A, $\hat{A}$, J_n, I_n and real powers of D. Let $\hat{M}$ be the matrix obtained by switching A and $\hat{A}$ in the definition of M. Then M and $\hat{M}$ have the same spectrum.

Proof. We follow the same proof presented by Godsil and McKay [26]. Define a matrix Q of order n as

$$Q = \left[\begin{array}{c|c} \frac{2}{s}J_s - I_s & \mathbf{0}_{s\times t} \\ \hline \mathbf{0}_{t\times s} & I_t \end{array}\right].$$

Then $Q = Q^{-1} = Q^T$. The sum of the entries in row i of A is equal to the sum of the entries in row i of $\hat{A}$. Given the structure of A, D has the form

$$D = \left[\begin{array}{c|c} (r + \frac{t_1}{2} + t_2)I_s & \mathbf{0}_{s\times t} \\ \hline \mathbf{0}_{t\times s} & \bar{D} \end{array}\right],$$

where $\bar{D}$ is a diagonal matrix of order t. For any $\alpha \in \mathbb{R}$, Q commutes with the matrix D^α, that is, $D^\alpha Q = QD^\alpha$. Also note that $QJ_n = J_nQ = J_n$ and $QAQ = \hat{A}$. Therefore, if M is any linear combination of products of nonnegative integer powers of A, $\hat{A}$, J_n, I_n and real powers of D, and $\hat{M}$ is the matrix obtained by switching A and $\hat{A}$ in the definition of M, then $QMQ = \hat{M}$. □

The phrase *GM switching* refers to the operation of replacing N in A with $J_{s\times t_1} - N$ to form $\hat{A}$. In the case that A is the adjacency matrix of a graph G, Theorem 2.5.1 allows us construct cospectral graphs with respect to the A, L, $|L|$, and $\mathcal{L}$-eigenvalues. This is because the matrix of degrees D will be the same for both the graph G with adjacency matrix A and the graph $\hat{G}$ with adjacency matrix $\hat{A}$ that results after GM switching (under the conditions of Theorem 2.5.1). Thus, if $\mathcal{L} = I - D^{-1/2}AD^{-1/2}$ is the normalized Laplacian of G, then $\hat{\mathcal{L}} = I - D^{-1/2}\hat{A}D^{-1/2}$ will be the normalized Laplacian of $\hat{G}$. However, in order to use Theorem 2.5.1 for graphs, there are many conditions that the graph must satisfy.

Let A be the adjacency matrix of a graph $G = (V, E)$ that satisfies the conditions in Theorem 2.5.1. Partition V the same way A is partitioned, that is, $V = S \cup T_1 \cup T_2 \cup T_3$, where S is the set of vertices of G corresponding to the columns of $A_{1,1}$, T_1 is the vertices of G corresponding to the columns of N, T_2 is the vertices of G corresponding to the columns of $J_{s\times t_2}$, and T_3 is the vertices of G corresponding to the columns of $0_{s\times t_3}$. Then for A to satisfy the conditions in Theorem 2.5.1 we require the following properties of G:

- The induced subgraph of G on the vertices in S must be regular.
- Each vertex in S must have the same degree in G.
- Each vertex in S must be adjacent to exactly half of the vertices in T_1.
- Each vertex in T_1 must be adjacent to exactly half of the vertices in S.
- Each vertex in T_2 must be adjacent to every vertex in S.
- Each vertex in T_3 must not be adjacent to any vertex in S.

Although these conditions are quite restrictive, we illustrate that Theorem 2.5.1 can produce many pairs of nonisomorphic non-regular cospectral graphs with respect to various matrix representations of graphs.

Example 2.5.2 *Consider $s = 4$ and $t_1 = 6$ in Theorem 2.5.1 and partition $V = S \cup T_1 \cup T_2 \cup T_3$ as above. Then the edges between S and T_1 must form a semiregular bipartite graph, where vertices in S are adjacent to 3 vertices of T_1 and vertices in T_1 are adjacent to 2 vertices of S. One such possibility is the subgraph on the left in Figure 2.2.*

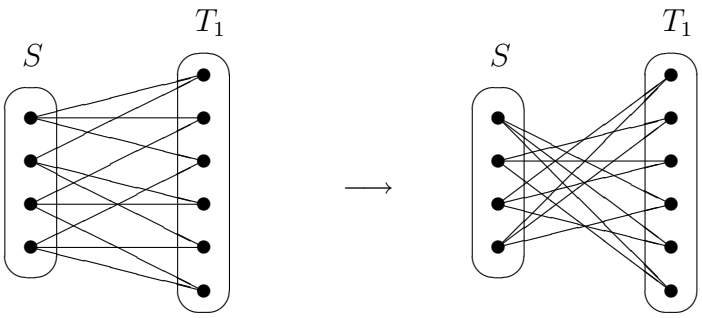

Figure 2.2: Using GM switching to generate cospectral graphs.

The edges of the graph on the left in Figure 2.2 represent the location of the 1's in N in the partition of A, and the edges of the graph on the right in Figure 2.2 represent the location of the 1's in $(J_{4\times 6} - N)$ in the partition of $\hat{A}$. What GM switching does is switches the edges and nonedges between S and T_1 while leaving the rest of the graph unchanged.

Let G be any graph with vertex partition $V = S \cup T_1 \cup T_2 \cup T_3$ that contains the graph on the left in Figure 2.2 as a subgraph on S and T_1 with $|S| = 4$ and $|T_1| = 6$, such that:

1. *There are exactly 12 edges between S and T_1 in G.*
2. *The induced subgraph of G on the vertices in S is regular.*
3. *Each vertex not in S or T_1 that is adjacent to a vertex in S is adjacent to every vertex in S.*

Form $\hat{G}$ by GM switching, that is, switch edges for nonedges between S and T_1, and keep the rest of the edges of G the same. Then by Theorem 2.5.1, the pair of graphs G and $\hat{G}$ are cospectral with respect to the A, L, $|L|$, and $\mathcal{L}$-eigenvalues.

One such example of a pair of nonismorphic non-regular graphs constructed using this technique is illustrated in Figure 2.3. The reason the two graphs in Figure 2.3 are nonisomorphic is because the graph on the left has a vertex adjacent to three vertices of degree 2, while the graph on the right does not.

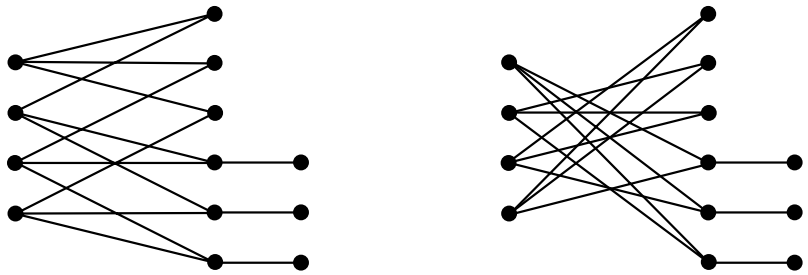

Figure 2.3: A pair of nonisomorphic non-regular cospectral graphs with respect to the A, L, $|L|$ and $\mathcal{L}$-eigenvalues.

Example 2.5.2 answers two questions that were asked by Butler in [9]. Figure 2.3 provides an example of two non-regular graphs which are cospectral with respect to the adjacency matrix, combinatorial Laplacian and normalized Laplacian at the same time. To construct graphs with arbitrarily high chromatic number that are cospectral with respect to the normalized Laplacian, we can start with Figure 2.2 and add vertices and edges as required without violating properties 1, 2, and 3 that are listed in Example 2.5.2, and then check if they are nonisomorphic. For example, attach a complete graph of order m to the bottom right degree 1 vertices of the graphs in Figure 2.3 and take m to be arbitrarily large.

2.6 Properties of graphs with exactly two or three distinct $\mathcal{L}$-eigenvalues

In this section we look at the structure of graphs which have exactly two or three distinct normalized Laplacian eigenvalues. In [19], van Dam and Haemers prove a nice result about the structure of graphs that have at most three distinct Laplacian eigenvalues.

Theorem 2.6.1 *[19] A connected graph G has at most three distinct L-eigenvalues if and only if there exist integers μ and $\bar{\mu}$, such that any two distinct nonadjacent vertices have exactly μ common neighbours, and any two adjacent vertices have exactly $\bar{\mu}$ common non-neighbours.*

In [19], van Dam and Haemers give a name to this a property. We say a non-complete graph G has *constant* $\mu = \mu(G)$ if any two vertices that are not adjacent have μ common neighbours. Further, G has *constant* μ *and* $\bar{\mu}$ if G has constant $\mu = \mu(G)$, and its complement

$\bar{G}$ has constant $\bar{\mu} = \mu(\bar{G})$. Thus, Theorem 2.6.1 says that a connected graph G has exactly three distinct L-eigenvalues if and only if G has constant μ and $\bar{\mu}$. Furthermore, a connected graph G has exactly two distinct L-eigenvalues if and only if G is the complete graph. To see that the complete graph is the only connected graph with exactly two distinct L-eigenvalues, let G be a connected graph on n vertices with Laplacian matrix L, and two distinct Laplacian eigenvalues 0 and λ. By the Cayley Hamilton Theorem, $(L - \lambda I)L = L(L - \lambda I) = \mathbf{0}$, from which it follows that every column of $L - \lambda I$ is a right null vector for L, and every row of $L - \lambda I$ is a left null vector for L. Hence $L - \lambda I = cJ$ for some scalar c, and we find that G must be complete.

It should be noted that graphs with constant μ and $\bar{\mu}$ generalize two known families of graphs. In the case that these graphs are regular then they are exactly the *strongly regular* graphs. In the case that $\mu = 1$ then we have the *geodetic graphs* of diameter two.

Since we will be dealing with strongly regular graphs below, we describe them here in more detail. Let G be a regular graph that is neither complete nor empty. Then G is *strongly regular* with *parameters* (n, k, a, c) if it is k-regular, every pair of adjacent vertices has a common neighbours, and every pair of distinct nonadjacent vertices has c common neighbours. The following feasibility condition is well known (see [27] for more details):

$$k(k - a - 1) = (n - k - 1)c.$$

It is also well known that a connected regular graph with exactly three distinct A-eigenvalues is strongly regular [27, Lemma 10.2.1]. A strongly regular graph with parameters

$$\left(n, \frac{n-1}{2}, \frac{n-5}{4}, \frac{n-1}{4}\right),$$

is called a *conference graph*. An example of a conference graph is a cycle on 5 vertices. Conference graphs are known to exist for small values of n that are allowed by the restrictions (such as, $n = 5,\ 9,\ 13,\ 17,\ 25,\ 29$), and also for prime powers congruent to 1 (modulo 4) (for example, *Paley graphs* [27]).

In an attempt to generalize Theorem 2.6.1, Wang, Fan and Tan [65] provide a condition that is equivalent for a connected graph having exactly t distinct L-eigenvalues (note that in the original statement of their result they omitted the word *nonzero*, which is necessary for the lemma to be true and thus is added here).

Lemma 2.6.2 *[65] Let G be a connected graph on $n \geq 3$ vertices and fix $2 \leq t \leq n$. Then G has exactly t distinct L-eigenvalues if and only if there exists $t - 1$ distinct nonzero numbers*

$\mu_1, \ldots, \mu_{t-1}$ *such that*

$$\prod_{i=1}^{t-1}(L - \mu_i I) = (-1)^{t-1}\frac{\prod_{i=1}^{t-1}\mu_i}{n}J.$$

Lemma 2.6.2 is a consequence of the Spectral Decomposition Theorem (along with minimal polynomials) and is a special case of a more general theorem for real symmetric matrices.

In particular, let M be a real symmetric matrix of order n. Let $\mu_1(M) < \cdots < \mu_t(M)$ be the distinct eigenvalues of M and take an orthonormal basis $\{x_1, \ldots, x_n\}$ of eigenvectors for M. For each fixed i, denote

$$P_i = x_{i_1}x_{i_1}^T + \cdots + x_{i_d}x_{i_d}^T,$$

where $\{x_{i_1}, \ldots, x_{i_d}\}$ is a basis of the eigenspace of $\mu_i(M)$ consisting of vectors from $\{x_1, \ldots, x_n\}$. The *Spectral Decomposition Theorem* says that

$$M = \sum_{i=1}^{t}\mu_i(M)P_i,$$

such that $P_i^2 = P_i = P_i^T$, for $1 \leq i \leq t$, and $P_iP_j = \mathbf{0}$, for $i \neq j$ (see [18] for more details). By the conditions on the P_i, for any polynomial f, we have,

$$f(M) = \sum_{i=1}^{t} f(\mu_i(M))P_i.$$

In particular, let f be the polynomial $f(x) = \prod_{i=2}^{t}(x - \mu_i(M))$. For $i \neq 1$, we have $f(\mu_i(M)) = 0$, and for $i = 1$ we have, $f(\mu_1(M)) = \prod_{i=2}^{t}(\mu_1(M) - \mu_i(M))$. Applying this to the normalized Laplacian where $\mu_1(\mathcal{L}) = 0$ gives the following result.

Lemma 2.6.3 *Let G be a connected graph on $n \geq 3$ vertices with m edges and fix $2 \leq t \leq n$. Then G has exactly t distinct $\mathcal{L}$-eigenvalues if and only if there exists $t-1$ distinct nonzero numbers $\mu_1, \ldots, \mu_{t-1}$ such that*

$$\prod_{i=1}^{t-1}(\mathcal{L} - \mu_i I) = (-1)^{t-1}\left(\prod_{i=1}^{t-1}\mu_i\right)\frac{D^{1/2}JD^{1/2}}{2m}, \tag{2.12}$$

where D is the matrix of degrees of G.

Proof. One direction is clear by the Spectral Decomposition Theorem and the fact that $D^{1/2}\mathbf{1}_n$ is an eigenvector of $\mathcal{L}$ with eigenvalue 0. For the other direction, multiply both sides of (2.12) by $\mathcal{L}$. This implies the minimal polynomial of $\mathcal{L}$ is

$$x(x - \mu_1)\cdots(x - \mu_{t-1}),$$

and hence $\mathcal{L}$ has exactly t distinct eigenvalues $0, \mu_1, \ldots, \mu_{t-1}$. □

A consequence of this is the following when $t = 2$.

Corollary 2.6.4 *Let G be a connected graph on $n \geq 3$ vertices. Then G has exactly two distinct $\mathcal{L}$-eigenvalues if and only if G is the complete graph.*

Let G be a connected graph of order n that has m edges and exactly three distinct $\mathcal{L}$-eigenvalues. Then by Lemma 2.6.3, there are two distinct nonzero numbers $\mu_1 < \mu_2$ such that

$$(\mathcal{L} - \mu_1 I)(\mathcal{L} - \mu_2 I) = \frac{\mu_1 \mu_2}{2m} D^{1/2} J D^{1/2}. \tag{2.13}$$

Hence, 0, μ_1, and μ_2 are the distinct eigenvalues of $\mathcal{L}$. Since G is not the complete graph, we have $0 < \mu_1 \leq 1$ and $\frac{n}{n-1} < \mu_2 \leq 2$. Suppose μ_1 (resp. μ_2) has multiplicity m_1 (resp. m_2). Then as G is connected we have,

$$m_1 + m_2 = n - 1,$$

and

$$m_1 \mu_1 + m_2 \mu_2 = n.$$

If $m_2 = 1$, then as $\mu_1 \leq 1$ we obtain $\mu_2 = 2$ and hence the graph is a bipartite graph. If a bipartite graph G is to have exactly three distinct $\mathcal{L}$-eigenvalues, by the symmetry about 1, the distinct $\mathcal{L}$-eigenvalues must be 0, 1 and 2. A connected graph G has $\mathcal{L}$-eigenvalues 0, 1 and 2 if and only if it is a complete bipartite graph. This follows from the result: G has only one positive A-eigenvalue if and only if G is a complete multipartite graph plus isolated vertices (see [17]).

By analyzing the entries of the matrices in (2.13), we have, for each i,

$$\sum_{k \in N_i} \frac{1}{d_k} = \frac{\mu_1 \mu_2}{2m} d_i^2 - (1 - \mu_1)(1 - \mu_2) d_i, \tag{2.14}$$

where N_i is the neighbourhood of i. For each pair of vertices i, j with $i \sim j$ in G,

$$\sum_{k \in N_i \cap N_j} \frac{1}{d_k} = \frac{\mu_1 \mu_2}{2m} d_i d_j + 2 - \mu_1 - \mu_2, \tag{2.15}$$

where in the case that $N_i \cap N_j = \emptyset$ the left side is 0. For each pair of vertices i, j with $i \not\sim j$ in G,

$$\sum_{k \in N_i \cap N_j} \frac{1}{d_k} = \frac{\mu_1 \mu_2}{2m} d_i d_j. \tag{2.16}$$

These three equations imply a number of things about the structure of a connected graph with three distinct $\mathcal{L}$-eigenvalues. For instance, any pair of nonadjacent vertices have at least one common neighbour by (2.16), implying the diameter of G is 2 (this also follows from a more general result that the diameter is at most one less than the number of distinct eigenvalues). Also, in the case the graph is regular, (2.15) and (2.16) imply that any two adjacent vertices have a constant number a of common neighbours, and any two distinct nonadjacent vertices have a constant number c of common neighbours, thus, the graph must be strongly regular (this also follows from noting that if G is regular with three distinct $\mathcal{L}$-eigenvalues, then it also has three distinct A-eigenvalues).

We summarize with the following remark.

Remark 2.6.5 *Let G be a connected graph of order n. Then the following statements hold.*

- *If G has exactly three distinct $\mathcal{L}$-eigenvalues then the diameter of G is 2.*
- *G has an $\mathcal{L}$-eigenvalue with multiplicity $n-2$ if and only if G is a complete bipartite graph.*
- *If G is bipartite then G has exactly three distinct $\mathcal{L}$-eigenvalues if and only if G is a complete bipartite graph.*
- *If G is regular then G has exactly three distinct $\mathcal{L}$-eigenvalues if and only if G is strongly regular.*

In [19], van Dam and Haemers show that in a graph with exactly three distinct L-eigenvalues only two distinct vertex degrees can occur. This is not the case for graphs with exactly three distinct $\mathcal{L}$-eigenvalues as we will see below. In the next result, we first look at the possibility of a vertex of degree 1 in the graph. An example of a graph satisfying condition (ii) of the next Theorem is illustrated in Figure 2.4, where H is taken to be a cycle on five vertices.

Theorem 2.6.6 *Let G be a connected graph of order $n \geq 3$ containing at least one vertex of degree 1. Then G has exactly three distinct $\mathcal{L}$-eigenvalues if and only if either*

(i) G is a star, or

(ii) there exists a conference graph H such that $G = \{u\} \vee (H \cup \{v\})$, that is, G is the join of a singleton vertex u with the union of a conference graph H and singleton vertex v.

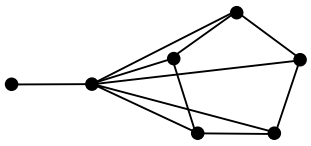

Figure 2.4: A graph with exactly three distinct $\mathcal{L}$-eigenvalues and three distinct vertex degrees.

Proof. Let $G = (V, E)$ be a graph of order n with m edges and $V = \{v_1, v_2, \ldots, v_n\}$. Suppose G has exactly three distinct $\mathcal{L}$-eigenvalues, namely, $0 < \mu_1 < \mu_2$. Without loss of generality, suppose v_1 is a vertex with degree 1 that is adjacent to v_2. Since the diameter of G is 2, we have that v_2 has degree $n-1$. Take any vertex $v_l \in V$, with $l \neq 1, 2$, and suppose v_l has degree d_l. Then by (2.16) with $i = v_1$ and $j = v_l$ we have

$$d_l = \frac{2m}{\mu_1\mu_2(n-1)},$$

implying that d_l is constant for each $l \neq 1, 2$, say $d_l = k$. Then, G has vertex degrees of 1, $n-1$ and k. If $k = 1$ then we have a star graph and G satisfies condition (i) of the theorem. Thus, let us suppose $k \neq 1$. We will use (2.14), (2.15) and (2.16) to derive a system of four equations. Using (2.14) with $i = v_1$, we obtain,

$$\frac{1}{n-1} = \frac{\mu_1\mu_2}{2m} - (1-\mu_1)(1-\mu_2).$$

Using (2.15) with $i = v_1$, $j = v_2$, we obtain,

$$0 = \frac{\mu_1\mu_2}{2m}(n-1) + 2 - \mu_1 - \mu_2.$$

Using (2.14) with $i = v_3$, we obtain,

$$\frac{1}{n-1} + \frac{k-1}{k} = \frac{\mu_1\mu_2}{2m}k^2 - (1-\mu_1)(1-\mu_2)k.$$

Using (2.16) with $i = v_1$, $j = v_3$, we obtain,

$$\frac{\mu_1\mu_2}{2m} = \frac{1}{k(n-1)}. \tag{2.17}$$

This system of four equations reduces to a system of three by using the substitution from (2.17) to replace the $\frac{\mu_1\mu_2}{2m}$ term in the first three equations:

$$(1-\mu_1)(1-\mu_2) = \frac{1-k}{k(n-1)}, \tag{2.18}$$

$$\mu_1 + \mu_2 - 2 = \frac{1}{k}, \tag{2.19}$$

$$(1-\mu_1)(1-\mu_2) = \frac{k^2 - k - (n-1)(k-1)}{k^2(n-1)}. \tag{2.20}$$

Then (2.18) and (2.20) allow us to solve for k in terms of n. We see that

$$2k^2 - (n+1)k + (n-1) = 0,$$

and hence, $k = 1$ or $k = \frac{n-1}{2}$. Thus, $k = \frac{n-1}{2}$. If u and v are vertices of degree k that are adjacent, then by (2.15) (along with (2.17) and (2.19)), u and v have

$$|N_u \cap N_v| = \frac{n-3}{4}$$

common neighbours. If u and v are vertices of degree k that are not adjacent, then by (2.16) (along with (2.17) and (2.19)), u and v have

$$|N_u \cap N_v| = \frac{n+1}{4}$$

common neighbours. Thus, using $N = n-2$, the induced subgraph of G on vertices $\{v_3, \ldots, v_n\}$ must be strongly regular with parameters

$$\left(N, \frac{N-1}{2}, \frac{N-5}{4}, \frac{N-1}{4}\right),$$

and hence, is a conference graph. Therefore, there is a conference graph H such that

$$G = \{v_2\} \vee (H \cup \{v_1\}).$$

We now show that the graphs listed in (i) and (ii) have three distinct $\mathcal{L}$-eigenvalues. If G is a star then G has three distinct eigenvalues of 0, 1 and 2, as mentioned in Example 1.6.2.

Suppose H is a conference graph on $n-2$ vertices and let $G = \{u\} \vee (H \cup \{v\})$ with degree matrix D. Note that $\mathcal{L}$ has exactly three distinct eigenvalues if and only if $D^{-1}A$ has exactly three distinct eigenvalues, since $D^{-1}A$ and $I - \mathcal{L}$ are similar. We will show that $D^{-1}A$ has exactly three distinct eigenvalues by constructing a set of n linearly independent eigenvectors. As H is a conference graph it has parameters

$$\left(n-2, \frac{n-3}{2}, \frac{n-7}{4}, \frac{n-3}{4}\right),$$

and so is regular of degree $\frac{n-3}{2}$. If H has one vertex then G is a star graph on 3 vertices. Thus, assume $n-2>1$ and so H is connected. The eigenvalues of the adjacency matrix of a strongly regular graph are well known (see [27]). Let $\hat{A}$ be the adjacency matrix of H with eigenvalues $\frac{n-3}{2}$, θ_1 and θ_2, where

$$\theta_1 = \frac{-1+\sqrt{n-2}}{2}, \text{ and } \quad \theta_2 = \frac{-1-\sqrt{n-2}}{2}.$$

We have that $\mathbf{1}_{n-2}$ is an eigenvector of $\hat{A}$ with eigenvalue $\frac{n-3}{2}$, and $\mathbf{1}_n$ is an eigenvector of $D^{-1}A$ with eigenvalue 1. Let $\{z_1, \ldots, z_{n-3}\}$ be the remaining eigenvectors of $\hat{A}$ such that $z_i \perp \mathbf{1}_{n-2}$. Note that

$$D^{-1}A = \left[\begin{array}{c|c|c} 0 & 1 & \mathbf{0}_{n-2}^T \\ \hline \frac{1}{n-1} & 0 & \frac{1}{n-1}\mathbf{1}_{n-2}^T \\ \hline \mathbf{0}_{n-2} & \frac{2}{n-1}\mathbf{1}_{n-2} & \frac{2}{n-1}\hat{A} \end{array}\right].$$

Then

$$D^{-1}A \left[\begin{array}{c} 0 \\ \hline 0 \\ \hline z_i \end{array}\right] = \frac{2\theta}{n-1} \left[\begin{array}{c} 0 \\ \hline 0 \\ \hline z_i \end{array}\right],$$

where θ is either θ_1 or θ_2. One can check that

$$\left[\begin{array}{c} a \\ \hline b_1 \\ \hline \mathbf{1}_{n-2} \end{array}\right], \qquad \left[\begin{array}{c} -a \\ \hline -b_2 \\ \hline \mathbf{1}_{n-2} \end{array}\right],$$

are eigenvectors for $D^{-1}A$ corresponding to eigenvalues $\frac{2\theta_2}{n-1}$ and $\frac{2\theta_1}{n-1}$ respectively, where

$$a = \frac{(n-1)\sqrt{n-2}}{2}, \; b_1 = \frac{2a\theta_2}{n-1}, \text{ and } b_2 = \frac{2a\theta_1}{n-1}.$$

Thus, we have a set of n linearly independent eigenvectors for $D^{-1}A$ with the three distinct eigenvalues

$$\left\{1, \frac{2\theta_1}{n-1}, \frac{2\theta_2}{n-1}\right\}.$$

□

Theorem 2.6.6 (ii) provides classes of graphs that have exactly three distinct $\mathcal{L}$-eigenvalues and three distinct vertex degrees, for example, see Figure 2.4 where H is taken to be a cycle on five vertices. We next provide some classes of graphs that have exactly three distinct $\mathcal{L}$-eigenvalues and two distinct vertex degrees.

Example 2.6.7 *Fix $s, m \geq 2$ and let G be the generalized petal graph $G = \{u\} \vee (sK_m)$, which is a generalization of the petal graph due to E. Wilmer (see [12, Example* 1.12*]). See Figure 2.5 for an illustration.*

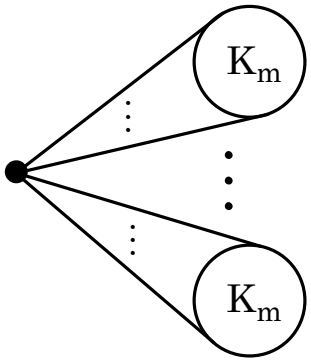

Figure 2.5: The generalized petal graph.

The $\mathcal{L}$-eigenvalues of G are

$$\left\{0^{(1)},\ \left(\frac{1}{m}\right)^{(s-1)},\ \left(\frac{m+1}{m}\right)^{(s(m-1)+1)}\right\}.$$

One simple way to prove this is to look at the block matrix

$$B = m(I - \mathcal{L}) + I = \left[\begin{array}{c|c|c|c|c} 1 & \frac{1}{\sqrt{s}}\mathbf{1}_m^T & \cdots & \cdots & \frac{1}{\sqrt{s}}\mathbf{1}_m^T \\ \hline \frac{1}{\sqrt{s}}\mathbf{1}_m & J_m & \mathbf{0}_m & \cdots & \mathbf{0}_m \\ \hline \vdots & \mathbf{0}_m & \ddots & \ddots & \vdots \\ \hline \vdots & \vdots & \ddots & \ddots & \mathbf{0}_m \\ \hline \frac{1}{\sqrt{s}}\mathbf{1}_m & \mathbf{0}_m & \cdots & \mathbf{0}_m & J_m \end{array}\right].$$

Take a set of vectors $\{\mathbf{1}_m, v_1, \ldots, v_{m-1}\}$ each of length m that form an orthonormal basis for $\mathbb{R}^m$. Then a set of linearly independent eigenvectors for B is

$$\left[\begin{array}{c} \sqrt{s} \\ \hline \mathbf{1}_m \\ \hline \vdots \\ \hline \mathbf{1}_m \end{array}\right], \left[\begin{array}{c} -m\sqrt{s} \\ \hline \mathbf{1}_m \\ \hline \vdots \\ \hline \mathbf{1}_m \end{array}\right], \left[\begin{array}{c} 0 \\ \hline \mathbf{1}_m \\ \hline -\mathbf{1}_m \\ \hline \mathbf{0}_m \\ \hline \vdots \\ \hline \mathbf{0}_m \end{array}\right], \ldots, \left[\begin{array}{c} 0 \\ \hline \mathbf{1}_m \\ \hline \mathbf{0}_m \\ \hline \vdots \\ \hline \mathbf{0}_m \\ \hline -\mathbf{1}_m \end{array}\right],$$

with corresponding eigenvalues $m+1$, 0, $m, \ldots, m$, *along with the* $s(m-1)$ *vectors*

$$\begin{bmatrix} 0 \\ \hline v_1 \\ \hline \mathbf{0}_m \\ \hline \vdots \\ \hline \mathbf{0}_m \end{bmatrix}, \ldots, \begin{bmatrix} 0 \\ \hline \mathbf{0}_m \\ \hline \vdots \\ \hline \mathbf{0}_m \\ \hline v_1 \end{bmatrix}, \ldots, \ldots, \ldots, \begin{bmatrix} 0 \\ \hline v_{m-1} \\ \hline \mathbf{0}_m \\ \hline \vdots \\ \hline \mathbf{0}_m \end{bmatrix}, \ldots, \begin{bmatrix} 0 \\ \hline \mathbf{0}_m \\ \hline \vdots \\ \hline \mathbf{0}_m \\ \hline v_{m-1} \end{bmatrix},$$

each with eigenvalue 0 *for* B. *Then* B *has eigenvalues* $(m+1)^{(1)}$, $0^{(s(m-1)+1)}$ *and* $m^{(s-1)}$, *from which the eigenvalues of* $\mathcal{L}$ *can be derived.*

Example 2.6.8 *Let* G *be the graph constructed as follows. Fix* $m \geq 1$. *Take the vertex set to be* $\{u_1, u_2, u_3, V_1, V_2, V_3\}$ *where each* V_i *is a set of* m *vertices, so that the graph has a total of* $3(m+1)$ *vertices. Let* G *have the edge set*

$$\{u_1x : x \in V_1 \cup V_2\} \cup \{u_2x : x \in V_1 \cup V_3\} \cup \{u_3x : x \in V_2 \cup V_3\} \cup$$

$$\{u_1u_2, u_2u_3, u_1u_3\} \cup \bigcup_{i=1}^{3} \{xy : x, y \in V_i, x \neq y\}.$$

See Figure 2.6 for an illustration.

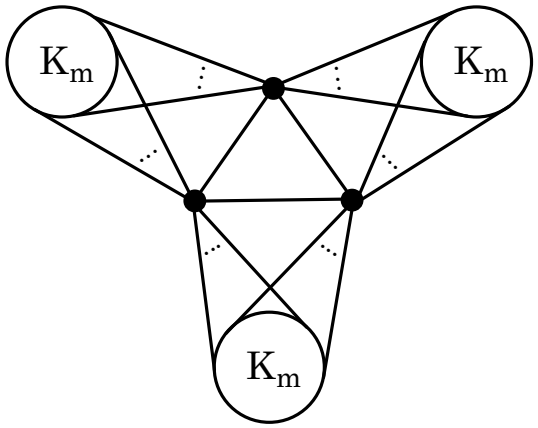

Figure 2.6: A graph with exactly three distinct $\mathcal{L}$*-eigenvalues and two distinct vertex degrees.*

Then G *has* $\mathcal{L}$*-eigenvalues*

$$\left\{0^{(1)}, \ \left(\frac{3}{2(m+1)}\right)^{(2)}, \ \left(\frac{m+2}{m+1}\right)^{(3m)}\right\}.$$

To show this, consider the block matrix

$$B = (m+1)\left(I - \mathcal{L} + \frac{1}{m+1}I\right)$$

$$= \left[\begin{array}{ccc|c|c|c} 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}}\mathbf{1}_m^T & \frac{1}{\sqrt{2}}\mathbf{1}_m^T & \mathbf{0}_m^T \\ \frac{1}{2} & 1 & \frac{1}{2} & \frac{1}{\sqrt{2}}\mathbf{1}_m^T & \mathbf{0}_m^T & \frac{1}{\sqrt{2}}\mathbf{1}_m^T \\ \frac{1}{2} & \frac{1}{2} & 1 & \mathbf{0}_m^T & \frac{1}{\sqrt{2}}\mathbf{1}_m^T & \frac{1}{\sqrt{2}}\mathbf{1}_m^T \\ \hline \frac{1}{\sqrt{2}}\mathbf{1}_m & \frac{1}{\sqrt{2}}\mathbf{1}_m & \mathbf{0}_m & J_m & \mathbf{0}_m & \mathbf{0}_m \\ \hline \frac{1}{\sqrt{2}}\mathbf{1}_m & \mathbf{0}_m & \frac{1}{\sqrt{2}}\mathbf{1}_m & \mathbf{0}_m & J_m & \mathbf{0}_m \\ \hline \mathbf{0}_m & \frac{1}{\sqrt{2}}\mathbf{1}_m & \frac{1}{\sqrt{2}}\mathbf{1}_m & \mathbf{0}_m & \mathbf{0}_m & J_m \end{array}\right].$$

We know 0 *is an eigenvalue of* $\mathcal{L}$*. We find a set of* $3m+2$ *linearly independent eigenvectors for* B *with the remaining eigenvalues. Take a set of vectors* $\{\mathbf{1}, v_1, \ldots, v_{m-1}\}$ *each of length* m *that form an orthonormal basis for* $\mathbb{R}^m$*. Then the* $3(m-1)$ *vectors*

$$\left[\begin{array}{c} 0 \\ 0 \\ 0 \\ \hline v_1 \\ \hline \mathbf{0}_m \\ \hline \mathbf{0}_m \end{array}\right], \left[\begin{array}{c} 0 \\ 0 \\ 0 \\ \hline \mathbf{0}_m \\ \hline v_1 \\ \hline \mathbf{0}_m \end{array}\right], \left[\begin{array}{c} 0 \\ 0 \\ 0 \\ \hline \mathbf{0}_m \\ \hline \mathbf{0}_m \\ \hline v_1 \end{array}\right], \ldots, \ldots, \ldots \left[\begin{array}{c} 0 \\ 0 \\ 0 \\ \hline v_{m-1} \\ \hline \mathbf{0}_m \\ \hline \mathbf{0}_m \end{array}\right], \left[\begin{array}{c} 0 \\ 0 \\ 0 \\ \hline \mathbf{0}_m \\ \hline v_{m-1} \\ \hline \mathbf{0}_m \end{array}\right], \left[\begin{array}{c} 0 \\ 0 \\ 0 \\ \hline \mathbf{0}_m \\ \hline \mathbf{0}_m \\ \hline v_{m-1} \end{array}\right],$$

are eigenvectors of B *each with eigenvalue* 0*. The two vectors*

$$\left[\begin{array}{c} 0 \\ 1 \\ -1 \\ \hline \sqrt{2}\ \mathbf{1}_m \\ \hline -\sqrt{2}\ \mathbf{1}_m \\ \hline \mathbf{0}_m \end{array}\right], \left[\begin{array}{c} -2 \\ 1 \\ 1 \\ \hline \sqrt{2}\ \mathbf{1}_m \\ \hline -\sqrt{2}\ \mathbf{1}_m \\ \hline -2\sqrt{2}\ \mathbf{1}_m \end{array}\right],$$

are eigenvectors of B *each with eigenvalue* $(2m+1)/2$*, and the vectors*

$$\left[\begin{array}{c} -1 \\ -1 \\ 1 \\ \hline \frac{\sqrt{2}}{m}\ \mathbf{1}_m \\ \hline \mathbf{0}_m \\ \hline \mathbf{0}_m \end{array}\right], \left[\begin{array}{c} -1 \\ 1 \\ -1 \\ \hline \mathbf{0}_m \\ \hline \frac{\sqrt{2}}{m}\ \mathbf{1}_m \\ \hline \mathbf{0}_m \end{array}\right], \left[\begin{array}{c} 1 \\ -1 \\ -1 \\ \hline \mathbf{0}_m \\ \hline \mathbf{0}_m \\ \hline \frac{\sqrt{2}}{m}\ \mathbf{1}_m \end{array}\right],$$

are eigenvectors of B each with eigenvalue 0. It is easy to see that these $3m+2$ vectors (along with the scaled and translated null vector for $\mathcal{L}$) are linearly independent.

Let G be a connected graph of order n with m edges. Suppose G has exactly three distinct $\mathcal{L}$-eigenvalues $0 < \mu_1 < \mu_2$ and two distinct vertex degrees d_A and d_B. Partition the vertex set as $A \cup B$ so that vertices in A have degree d_A and vertices in B have degree d_B. Then (2.14) implies that for every $x \in A$, we have

$$e(x, B) = \frac{e(A, B)}{|A|},$$

and for every $x \in B$, we have

$$e(x, A) = \frac{e(A, B)}{|B|}.$$

Thus, the edges between A and B form a semiregular bipartite graph. The graphs in Examples 2.6.7 and 2.6.8 are cases where exactly two vertex degrees occur and thus satisfy the above condition. By Remark 2.4.6, we have

$$\mu_2 = e(A, B)\left(\frac{1}{|A|d_A} + \frac{1}{|B|d_B}\right).$$

Then,

$$\mu_1 = \frac{(\mu_2 - 1)|A||B|}{e(A, B)}.$$

Note that we can rewrite μ_2 as

$$\mu_2 = \frac{2m \cdot e(A, B)}{|A||B|d_A d_B}.$$

It would be interesting to know what this implies about the structure of G. Since the edges between A and B form a semiregular bipartite graph, we know that the induced subgraph of G on A and the induced subgraph of G on B both need to be regular, however, must they be strongly regular, empty, or complete?

For graphs of orders $3 \leq n \leq 10$, Matlab was used to find all connected graphs of order n with exactly three distinct $\mathcal{L}$-eigenvalues by using a database of nonisomorphic connected graphs (in particular, [48]). The graphs found are complete bipartite graphs, strongly regular graphs, graphs from the families listed in Examples 2.6.7, 2.6.8 and Theorem 2.6.6, along with an additional graph that does not fall under one of these families (see Figure 2.7).

For $n = 3$, there is one graph: $K_{1,2}$.

For $n = 4$, there are two graphs: $K_{1,3}$ and $K_{2,2}$.

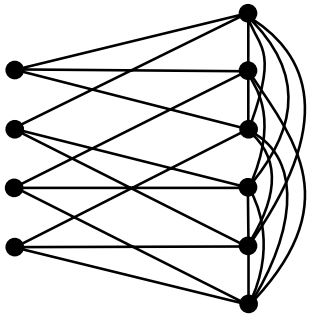

Figure 2.7: A graph on 10 vertices with exactly three distinct $\mathcal{L}$-eigenvalues.

For $n = 5$, there are four graphs: $K_{1,4}$, $K_{2,3}$, C_5 and $\{u\} \vee (2K_2)$.

For $n = 6$, there are five graphs: $K_{1,5}$, $K_{2,4}$, $K_{3,3}$, $K_{2,2,2}$ and the graph in Example 2.6.8 with $m = 1$.

For $n = 7$, there are six graphs: $K_{1,6}$, $K_{2,5}$, $K_{3,4}$, $\{u\} \vee (3K_2)$, $\{u\} \vee (2K_3)$, and $\{u\} \vee (C_5 \cup \{v\})$.

For $n = 8$, there are five graphs: $K_{1,7}$, $K_{2,6}$, $K_{3,5}$, $K_{4,4}$ and $K_{2,2,2,2}$.

For $n = 9$, there are nine graphs: $K_{1,8}$, $K_{2,7}$, $K_{3,6}$, $K_{4,5}$, $\{u\} \vee (4K_2)$, $\{u\} \vee (2K_4)$, $K_{3,3,3}$, the generalized quadrangle $GQ(2, 1)$ (which is a strongly regular graph, see [27]), and the graph in Example 2.6.8 with $m = 2$.

For $n = 10$, there are ten graphs: $K_{1,9}$, $K_{2,8}$, $K_{3,7}$, $K_{4,6}$, $K_{5,5}$, $K_{2,2,2,2,2}$, the Petersen graph, $\{u\} \vee (3K_3)$, the 5-triangular graph (which is a strongly regular graph, see [27]), and the graph in Figure 2.7. Note that the graph in Figure 2.7 has $K_{2,2,2}$ (which is strongly regular) as an induced subgraph of the vertices on the right side part.

Finally, we remark that not all graphs with constant μ and $\bar{\mu}$ have exactly three distinct $\mathcal{L}$-eigenvalues, though they have exactly three distinct L-eigenvalues (see Theorem 2.6.1). For example, consider the graph G formed by removing a single edge from K_4. Then G has constant $\mu = 2$ and $\bar{\mu} = 0$, thus, has exactly three distinct L-eigenvalues. However, G has four distinct $\mathcal{L}$-eigenvalues.

2.7 Relationship to the general Randić index $R_{-1}(G)$

We begin with two other formulations of $R_{-1}(G)$. By analyzing the entries in $(I-\mathcal{L})^2$ and using (1.5), observe that

$$tr((I-\mathcal{L})^2) = 2\sum_{x\sim y}\frac{1}{d_x d_y} = 2R_{-1}(G).$$

Hence,

$$R_{-1}(G) = \frac{tr((I-\mathcal{L})^2)}{2}. \tag{2.21}$$

Also, observe that using (2.21) and the fact that $tr(\mathcal{L}) = n$ we can derive

$$R_{-1}(G) = \frac{1}{2}\mathbf{1}^T D^{-1}AD^{-1}\mathbf{1}. \tag{2.22}$$

In the next lemma we see the importance of $R_{-1}(G)$ when analyzing the $\mathcal{L}$-energy of a graph.

Lemma 2.7.1 *Let G be a graph of order n with no isolated vertices. Then*

$$2R_{-1}(G) \leq E_{\mathcal{L}}(G) \leq \sqrt{2nR_{-1}(G)}.$$

Proof. As mentioned in Section 1.8, by the Cauchy-Schwarz inequality with (1.2) (using vectors $(1,\ldots,1)^T$ and $(|\lambda_1(I-\mathcal{L})|,\ldots,|\lambda_n(I-L)|)^T$) along with (2.21) we obtain the upper bound

$$E_{\mathcal{L}}(G) \leq \sqrt{n\sum_{i=1}^{n}[\lambda_i(I-\mathcal{L})]^2} = \sqrt{n\cdot tr((I-\mathcal{L})^2)} = \sqrt{2nR_{-1}(G)}.$$

Note that the eigenvalues of $I-\mathcal{L}$ lie in the interval $[-1,1]$. Thus, $[\lambda_i(I-\mathcal{L})]^2 \leq |\lambda_i(I-\mathcal{L})|$, giving,

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{n}|\lambda_i(I-\mathcal{L})| \geq \sum_{i=1}^{n}[\lambda_i(I-\mathcal{L})]^2 = tr((I-\mathcal{L})^2) = 2R_{-1}(G).$$

□

Thus, determining how the structure of a graph relates to $R_{-1}(G)$ will provide information about $E_{\mathcal{L}}(G)$. It should be noted that $R_{-1}(G)$ comes up in other ways when analyzing the eigenvalues of $\mathcal{L}$. In [10], Butler provides a bound on the gap between the nontrivial largest and smallest eigenvalues of $\mathcal{L}$ in terms of formulation (2.22) of $R_{-1}(G)$. We restate this result using $R_{-1}(G)$.

Lemma 2.7.2 *[10, Corollary 9] Let G be a connected graph of order n with normalized Laplacian matrix $\mathcal{L}$. Then*

$$\sqrt{\frac{\lambda_n(\mathcal{L})}{\lambda_2(\mathcal{L})}} + \sqrt{\frac{\lambda_2(\mathcal{L})}{\lambda_n(\mathcal{L})}} \geq 2\sqrt{\left(1-\frac{1}{n}\right)\left(1+\frac{2}{n}R_{-1}(G)\right)}.$$

and

$$\lambda_n(\mathcal{L}) - \lambda_2(\mathcal{L}) \geq \frac{2}{n-1}\sqrt{2(n-1)R_{-1}(G) - n}.$$

In [12, Equation 1.9], Chung defines

$$\overline{\lambda} = \max_{i \neq 1} |1 - \lambda_i(\mathcal{L})|,$$

which appears when dealing with random walks on graphs. Then (as in [12]) we have

$$\begin{aligned} tr(I-\mathcal{L})^2 &= \sum_{i=1}^{n}(1-\lambda_i(\mathcal{L}))^2, \\ &\leq 1 + (n-1)\overline{\lambda}^2, \end{aligned}$$

and using formulation (2.21) of $R_{-1}(G)$ we can rewrite this as

$$R_{-1}(G) \leq \frac{1+(n-1)\overline{\lambda}^2}{2}.$$

Also, in [67, Lemma 2.33] the notation $e_{-1}(G,G)$ is used which is equal to $2R_{-1}(G)$. In [25], the authors bound $R_{-1}(G)$ in terms of n, $\lambda_n(\mathcal{L})$ and $\lambda_2(\mathcal{L})$.

Theorem 2.7.3 *[25, Theorem 1.1] Let G be a connected graph on n vertices. Then*

$$R_{-1}(G) \leq \frac{1}{2}(n-1)(n-2)\left(\lambda_n(\mathcal{L}) - \frac{n}{n-1}\right)^2 + \frac{n}{2(n-1)},$$

$$R_{-1}(G) \leq \frac{1}{2}(n-1)(n-2)\left(\lambda_2(\mathcal{L}) - \frac{n}{n-1}\right)^2 + \frac{n}{2(n-1)},$$

with equalities holding if and only if G is the complete graph.

If G is a graph of order n, we will see in the next section that $\binom{n}{2} - R_{-1}(G)$ appears as a coefficient in the characteristic polynomial of $\mathcal{L}$. Thus, when studying eigenvalues of $\mathcal{L}$, the general Randić index $R_{-1}(G)$ is an important parameter. In Chapter 3, we will look at upper and lower bounds on $R_{-1}(G)$ in more detail.

2.8 Results of Runge

Fritz Runge was a doctoral student of H. Sachs during the 1970's. His dissertation, which is in German, deals with contributions to the theory of spectra of graphs and hypergraphs. A consequence of his results is a "Matrix-Tree Theorem" and a "Coefficients Theorem" for the normalized Laplacian. Additionally, the general Randić index $R_{-1}(G)$ (indirectly) appeared in one of his results which led to a (now settled) conjecture relating $R_{-1}(G)$ with the number of edges of G and the largest A-eigenvalue of G (called the *index* of a graph). This section is meant to give credit to Runge and make mention of his contributions regarding the spectrum of $\mathcal{L}$.

In fact, Runge did not deal directly with $\mathcal{L}$ but rather with the matrix $Q = D^{-1}A$. Since

$$Q = D^{-1}A = D^{-1/2}(I - \mathcal{L})D^{1/2},$$

we see that Q and $I - \mathcal{L}$ are similar. Thus, for any graph, Q and $I - \mathcal{L}$ have the same eigenvalues and the same characteristic polynomial. In his dissertation, Runge proves a number of results about the characteristic polynomial of Q which must also hold for the characteristic polynomial of $I - \mathcal{L}$. Throughout this section, we rephrase some of the results of Runge in terms of the spectrum of $\mathcal{L}$. It should be noted that the matrix $\frac{1}{2}(Q + I)$ and its spectrum are important in Correspondence Analysis [59].

One classical combinatorial result is the Matrix-Tree Theorem which states that the determinant of any cofactor of the combinatorial Laplacian L is equal to the number of spanning trees in a graph. Hence, the number of spanning trees of a graph G is given by

$$t(G) = \frac{1}{n}\prod_{i=2}^{n}\lambda_i(L).$$

Runge and Sachs [57, 58] proved a similar result for the spectrum of Q, which we rephrase for $\mathcal{L}$.

Theorem 2.8.1 *[17, Section* 1.9 #10*] Let G be a graph of order n with degree matrix D. Then the number of spanning trees of G is given by*

$$t(G) = \frac{\det D}{\operatorname{vol} G}\prod_{i=2}^{n}\lambda_i(\mathcal{L}).$$

Runge and Sachs [57] then generalize this result to obtain an analogous formula for the number of "total spanning trees" in a hypergraph.

Runge also listed two formulas for the coefficients of the characteristic polynomial of Q. One in terms of the cycle structure of the graph, and another in terms of the tree structure. Suppose Q has characteristic polynomial

$$\det(\lambda I - Q) = q_0\lambda^n + q_1\lambda^{n-1} + \cdots + q_{n-1}\lambda + q_n,$$

and $\mathcal{L}$ has characteristic polynomial

$$\det(\lambda I - \mathcal{L}) = c_0\lambda^n + c_1\lambda^{n-1} + \cdots + c_{n-1}\lambda + c_n,$$

where $c_0 = q_0 = 1$. By the Binomial Theorem, the following relationship holds between the coefficients of the characteristic polynomial of Q and that of $\mathcal{L}$:

$$c_{n-k} = \sum_{i=0}^{n-k}(-1)^{n+k}\binom{n-i}{k}q_i \quad \text{and} \quad q_{n-k} = \sum_{i=0}^{n-k}(-1)^{n+k}\binom{n-i}{k}c_i.$$

It can easily be determined that $q_2 = -R_{-1}(G)$. We also have the following information about c_i:

$$c_1 = -n, \qquad c_2 = \binom{n}{2} - R_{-1}(G), \qquad c_{n-1} = \frac{(-1)^{n-1}\operatorname{vol} G}{\det D}\ t(G), \qquad c_n = 0.$$

Before we list Runge's formula for q_i in terms of the tree structure, we require some notation. Let $G = (V, E)$ be a graph of order n. Let $J = \{j_1, j_2, \ldots, j_q\} \subseteq V$. For $J \neq \emptyset$, we let G_J denote the multigraph obtained from G by identifying the vertices $j_1, j_2, \ldots, j_q$, thereby replacing the set $\{j_1, j_2, \ldots, j_q\}$ by a single new vertex v. The number of loops on v is equal to the number of edges in the induced subgraph of G on J, and the number of edges from v to k, for $k \in V\backslash J$, is equal to the number of $j \in J$ such that jk is an edge in G. Thus, this identification creates a new multigraph G_J that contains both loops and multiple edges. Note that if $|J| = 1$, then $G_J = G$. The notion of spanning trees is easily extended to that of multigraphs. We let $t(G_J)$ denote the number of spanning trees in the multigraph G_J, and we use the convention that $t(G_V) = 1$. Runge proved the following formula for the coefficients of the characteristic polynomial of Q.

Theorem 2.8.2 *[17, Theorem 1.5] Let G be a graph without isolated vertices and $Q = D^{-1}A$, where D is the matrix of degrees. If Q has characteristic polynomial*

$$\det(\lambda I - Q) = q_0\lambda^n + q_1\lambda^{n-1} + \cdots + q_{n-1}\lambda + q_n,$$

then for $i = 0, 1, \ldots, n$,

$$q_i = (-1)^{n-i} \sum_{j=n-i}^{n} \binom{j}{n-i} (-1)^j \sum_{\substack{J \subseteq V \\ |J|=j}} \frac{t(G_J)}{\prod_{k \in V \setminus J} d_k},$$

where the conventions $t(G_\emptyset) = 0$ *and* $\prod_{k \in \emptyset} d_k = 1$ *are adopted.*

From this, we can deduce the coefficients of the characteristic polynomial of $\mathcal{L}$ in terms of the tree structure of the graph.

Corollary 2.8.3 *Let* G *be a graph without isolated vertices. If* $\mathcal{L}$ *has characteristic polynomial*

$$\det(\lambda I - \mathcal{L}) = c_0 \lambda^n + c_1 \lambda^{n-1} + \cdots + c_{n-1} \lambda + c_n,$$

then for $i = 0, 1, \ldots, n$,

$$c_{n-i} = (-1)^{(n-i)} \sum_{\substack{J \subseteq V \\ |J|=i}} \frac{t(G_J)}{\prod_{k \in V \setminus J} d_k},$$

where the conventions $t(G_\emptyset) = 0$ *and* $\prod_{k \in \emptyset} d_k = 1$ *are adopted.*

Runge also provided a formula for the coefficients of the characteristic polynomial of Q in terms of the cycle structure of a graph that can also be interpreted in terms of $\mathcal{L}$. We omit the formulas here and remark that they can be found in [17, Theorem 1.5*a*].

In 1996, an analog of the Matrix-Tree Theorem was proved by Chung and Langlands [13] for a combinatorial Laplacian with vertex weights (for which $\mathcal{L}$ is a special case by using weights $\frac{1}{d_x}$). They looked at rooted directed spanning forests rather than a multigraph G_J, although these two notions are similar in flavour. Let $G = (V, E)$ be a graph of order n. Let S denote a subset of vertices with $|S| = s$ and X denote a subset of $n - s$ edges. If the subgraph with vertex set V and edge set X is a spanning forest and each of the subtrees contains exactly one vertex in S, we can then define the *rooted directed spanning forest* X_S which consists of all edges of X oriented toward S. For a rooted directed spanning forest X_S, we define the *weight of* X_S as follows:

$$\omega(X_S) = \prod_{(x,y) \in E(X_S)} \frac{1}{d_y}$$

and

$$\kappa_S(G) = \sum_{X_S} \omega(X_S).$$

Chung and Langlands [13] proved the following for the coefficients of the characteristic polynomial of a vertex weighted Laplacian, which we restate for $\mathcal{L}$ and c_{n-i}.

Theorem 2.8.4 *[13, Theorem 2] Let $G = (V, E)$ be a graph without isolated vertices. If $\mathcal{L}$ has characteristic polynomial*

$$\det(\lambda I - \mathcal{L}) = c_0\lambda^n + c_1\lambda^{n-1} + \cdots + c_{n-1}\lambda + c_n,$$

then for $i = 0, 1, \ldots, n$,

$$c_{n-i} = (-1)^{(n-i)} \sum_{\substack{S \subseteq V \\ |S|=n-i}} \kappa_S(G).$$

As seen in Example 1.6.6, if G is a regular graph of degree r then

$$\mathcal{L} = I - \frac{1}{r}A.$$

Runge also showed that the Q-eigenvalues can be determined from the A-eigenvalues in the case that G is a regular graph. Additionally, he showed the Q-eigenvalues can be determined from the A-eigenvalues in the case that G is a semiregular bipartite graph.

Remark 2.8.5 *[17, Theorem 1.1] If G is a regular graph of degree r, then for each $1 \leq i \leq n$,*

$$\lambda_i(\mathcal{L}) = 1 - \frac{1}{r}\lambda_{n-i+1}(A).$$

If G is a semiregular bipartite graph of degrees r_1 and r_2, then for each $1 \leq i \leq n$,

$$\lambda_i(\mathcal{L}) = 1 - \frac{1}{\sqrt{r_1 r_2}}\lambda_{n-i+1}(A).$$

Finally, we note that Runge (indirectly) dealt with the general Randić index $R_{-1}(G)$. Let $G = (V, E)$ be a graph of order n with no isolated vertices and m edges. Then Runge showed

$$\sum_{i=1}^{n} \lambda_i^2(Q) = 2\sum_{x \sim y} \frac{1}{d_x d_y}.$$

A consequence of this is the following, which we restate in terms of $R_{-1}(G)$. Note that if G is a graph, then we call $\lambda_n(A)$ the *index* of G and denote by ρ.

Corollary 2.8.6 *[17, Section 1.9 #8] Let G be a graph of order n with no isolated vertices and m edges. Suppose G is a regular graph of degree r (resp. semiregular bipartite graph of degrees r_1 and r_2). Let ρ be the index of G, that is, $\rho = r$ (resp. $\rho = \sqrt{r_1 r_2}$). Then*

$$m = \rho^2 R_{-1}(G). \tag{2.23}$$

Runge then asked if (2.23) is sufficient for a graph to be either regular or semiregular [17, Section 1.9 #8]. This was shown to be false by Hofmeister [35] who proposed a modified conjecture. We first require a definition. Let G be a graph of order n with no isolated vertices. Then G is called *almost regular* if there is a nonnegative real number r such that every component of G is either r-regular or semiregular bipartite with degrees r_1 and r_2 with $r_1 r_2 = r^2$. Hofmeister [35] conjectured that the condition in (2.23) is sufficient for a graph to be almost regular. Later, Hoffman, Hofmeister and Wolfe [34] proved a generalization of this modified conjecture. Then Simić and Stevanović provided a shorter proof for the theorem in [62]. We restate the theorem in terms of $R_{-1}(G)$.

Theorem 2.8.7 *[34, 62] For any graph G with no isolated vertices, m edges and index ρ, we have*

$$\rho^2 \geq \frac{m}{R_{-1}(G)}.$$

Equality holds if and only if G is almost regular.

3 THE GENERAL RANDIĆ INDEX

3.1 Introduction

In this chapter, we first highlight some relevant results on the parameter $R_{-1}(G)$ that have independently appeared in the literature. Many of the results known for $R_{-1}(G)$ are for trees and chemical graphs, that is, graph representations of chemical compounds. See [17, Chapter 8] for more details on relating chemistry to graph theory. Here, we extend an upper bound on $R_{-1}(G)$ known to be true for trees to connected graphs. We also discuss how $R_{-1}(G)$ can change when an edge is deleted from G.

3.2 Upper and lower bounds on $R_{-1}(G)$

We first provide a few bounds on $R_{-1}(G)$ in terms of other graph parameters. By considering the minimum and maximum degrees of G, we obtain upper and lower bounds on $R_{-1}(G)$.

Theorem 3.2.1 *Let G be a graph of order n with no isolated vertices. Suppose G has minimum vertex degree equal to $d_{\min}$ and maximum vertex degree equal to $d_{\max}$. Then*

$$\frac{n}{2d_{\max}} \leq R_{-1}(G) \leq \frac{n}{2d_{\min}}.$$

Equality occurs in both bounds if and only if G is a regular graph.

Proof. By (1.7) we have,

$$\begin{aligned} R_{-1}(G) &\leq \frac{1}{2}\sum_{y\in V}\frac{1}{d_y}\sum_{\substack{x\\ x\sim y}}\frac{1}{d_{\min}}, \\ &= \frac{1}{2}\sum_{y\in V}\frac{1}{d_y}\frac{d_y}{d_{\min}}, \\ &= \frac{n}{2d_{\min}}. \end{aligned}$$

Similarly,

$$\begin{aligned} R_{-1}(G) &\geq \frac{1}{2}\sum_{y\in V}\frac{1}{d_y}\sum_{\substack{x\\ x\sim y}}\frac{1}{d_{\max}}, \\ &= \frac{n}{2d_{\max}}. \end{aligned}$$

It is easy to see that equality occurs in both bounds if and only if G is a regular graph. □

It should be noted that in [61, Theorem 2.2 & 2.3] an analogous result to Theorem 3.2.1 on $R_\alpha(G)$ was presented independently by Shi when taking $\alpha = -1$.

The next result provides bounds on $R_{-1}(G)$ strictly in terms of the order of G. Recall that the *length* of a path is the number of edges that the path uses. It should be noted that an analogous result to the next Theorem was stated independently by Li and Yang [43, Theorem 3.2].

Theorem 3.2.2 *Let G be a graph of order n with no isolated vertices. Then*

$$\frac{n}{2(n-1)} \leq R_{-1}(G) \leq \left\lfloor \frac{n}{2} \right\rfloor,$$

with equality in the lower bound if and only if G is a complete graph, and equality in the upper bound if and only if either

(i) n is even and G is the disjoint union of $n/2$ paths of length 1, or

(ii) n is odd and G is the disjoint union of $(n-3)/2$ paths of length 1 and one path of length 2.

Proof. The lower bound follows from Theorem 3.2.1 as $d_{\max} \leq n-1$, and equality occurs if and only if G is regular of degree $n-1$, hence, complete.

If n is even, then the upper bound follows from Theorem 3.2.1 as $d_{\min} \geq 1$, and equality occurs if and only if G is regular of degree 1, hence, G is the disjoint union of $n/2$ paths of length 1.

If n is odd, then we will show that $R_{-1}(G) \leq \frac{n-1}{2}$. Since G has no isolated vertices, there is a vertex x with degree at least $d_x \geq 2$. Suppose that x is adjacent to $\{y_1, y_2, \ldots, y_{d_x}\}$. By

(1.7) we have,

$$\begin{aligned} R_{-1}(G) &\leq \frac{n-(d_x+1)}{2} + \frac{1}{2d_x}\sum_{i=1}^{d_x}\frac{1}{d_{y_i}} + \frac{1}{2}\sum_{i=1}^{d_x}\frac{1}{d_{y_i}}\left(\frac{1}{d_x} + \sum_{\substack{u\neq x\\ u\sim y_i}}\frac{1}{d_{\min}}\right), \\ &\leq \frac{n-1}{2} + \left(\frac{1}{d_x} - \frac{1}{2}\right)\left(\sum_{i=1}^{d_x}\frac{1}{d_{y_i}}\right), \\ &\leq \frac{n-1}{2}. \end{aligned}$$

It is easy to see that equality occurs if and only if there is one vertex of degree 2 and the other $n-1$ vertices have degree 1, that is, G is the disjoint union of $(n-3)/2$ paths of length 1 and one path of length 2. □

If G is a disconnected graph with k connected components, in particular,

$$G_1, \ldots, G_k,$$

then

$$R_{-1}(G) = \sum_{i=1}^{k} R_{-1}(G_i).$$

Thus, it is interesting to know how $R_{-1}(G)$ behaves for the class of connected graphs.

3.3 Bounds on $R_{-1}(G)$ over the class of connected graphs

One upper bound on $R_{-1}(G)$ when G is a connected graph comes from [45].

Lemma 3.3.1 *[45, Corollary 2] If G is a connected graph of order n, then*

$$R_{-1}(G) \leq \frac{1}{2}\sum_{i=1}^{n}\frac{1}{d_i}.$$

Equality occurs if and only if G is regular.

In [14], Clark and Moon provide bounds on $R_{-1}(T)$, for a tree T of order n. They showed that

$$1 \leq R_{-1}(T) \leq \frac{5n+8}{18}.$$

Clark and Moon [14] then proposed two problems:

1. Find $K = \lim_{n\to\infty} \frac{f(n)}{n}$, where $f(n)$ is the maximum value of $R_{-1}(T)$ among all trees T of order n.

2. Refine the upper bound for $R_{-1}(T)$ so that it is sharp for infinitely many values of n.

Hu, Li and Yuan [38] gave a first solution to both problems, however, gaps were found in their proof (see [51]). Then Pavlović, Stojanović and Li gave a sound proof in [52].

Theorem 3.3.2 *[38, 52] For a tree T of order $n \geq 103$,*

$$R_{-1}(T) \leq \frac{15n-1}{56}.$$

A class of trees is provided in [14] that satisfies equality in Theorem 3.3.2 for infinitely many values of n. Theorem 3.3.2 together with the result in [14] implies that $K = \frac{15}{56}$ in the first problem posed by Clark and Moon. See [53] for a further refinement giving a sharp upper bound for $R_{-1}(T)$ amongst all trees T of order n, for $n \geq 720$. Also, see [41, 42] for many other results concerning bounds for $R_{-1}(T)$. In what follows, we will see that the bound $R_{-1}(G) \leq \frac{15(n+1)}{56}$ holds for any connected graph G of order $n \geq 3$. This bound is not sharp for all n, and we suspect that a refined bound similar to that in [53] can be achieved with extra consideration.

We first provide some notation to help structure G. We say G has a *suspended path* from u to w, if uvw is a path with $d_u^G = 1$ and $d_v^G = 2$. Note that we don't require $d_w^G \geq 3$ as in [14].

A $(t, s+t)$*-system centered at* r is an induced subgraph of G, such that there are t suspended paths to vertex r and $d_r^G = s + t$. This is illustrated in Figure 3.1.

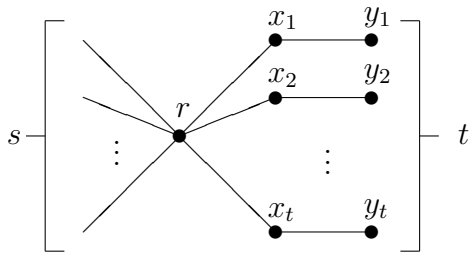

Figure 3.1: A $(t, s+t)$-system centered at r.

A $(k, t, s+k)$*-system centered at* R is an induced subgraph of G that has k vertex disjoint $(t, t+1)$-systems centered at $r_1, r_2, \ldots, r_k$, such that R is adjacent to each r_i and $d_R^G = s + k$. This is illustrated in Figure 3.2.

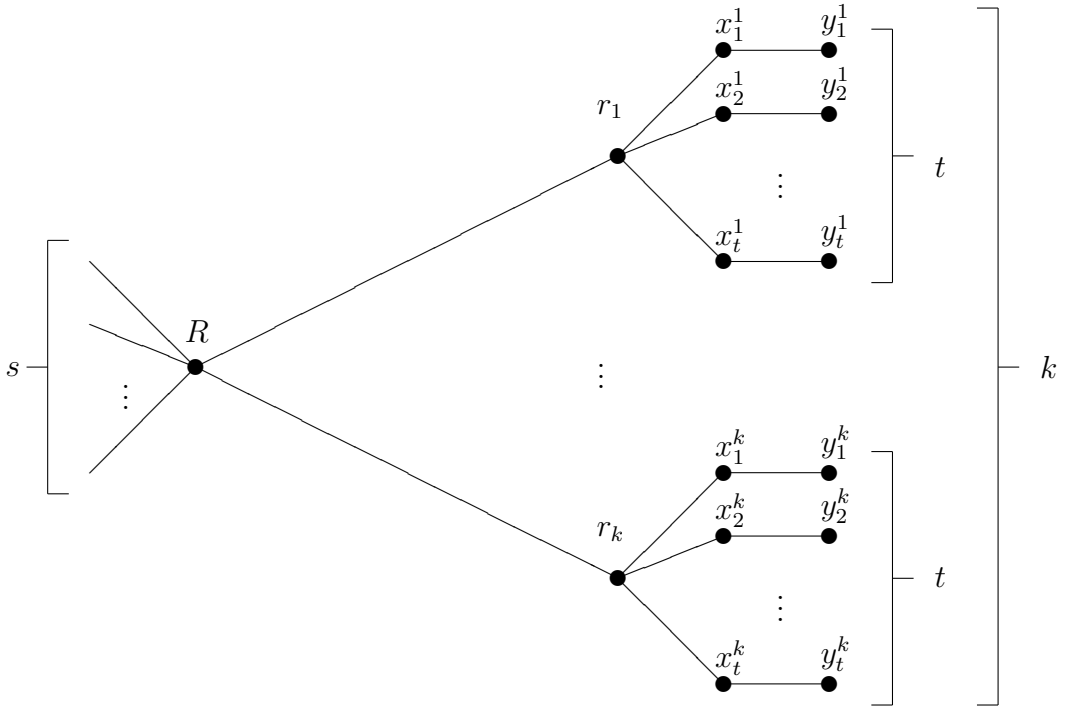

Figure 3.2: A $(k, t, s + k)$-system centered at R.

The set of all $(t, s + t)$-systems of G, for $s \geq 0$ and $t \geq 1$, and $(k, t, s + k)$-systems of G, for $s \geq 0$ and $k, t \geq 1$, is referred to as the *collection of systems* of G. Any object in this collection is referred to as a *system* of G. Note that a vertex z of G may be the center of many different systems.

One question to ask is if there is always a tree on n vertices that maximizes $R_{-1}(G)$ over all connected graphs of order n. If the answer is yes, then the bound for connected graphs would follow immediately. A first approach would be to look at the spanning trees of G and see if $R_{-1}(G) \leq R_{-1}(T)$ for some spanning tree T of G. However, it is interesting to note that there exist graphs G such that for every spanning tree T of G, the inequality $R_{-1}(T) < R_{-1}(G)$ holds.

Example 3.3.3 *Let G be the graph described as follows: Let $t > 16$ be a natural number and consider a cycle with 3 vertices a_1, a_2, a_3 each with degree 4 and with each of a_1, a_2, a_3 being the center of a $(2, t, 4)$-system. The order of G is $12t + 9$ and the only spanning trees of G are obtained by removing an edge on the cycle (namely, a_1a_2, a_2a_3 or a_1a_3). If T is*

any spanning tree of G then,

$$R_{-1}(G) - R_{-1}(T) = \left(\frac{1}{t} + \frac{3}{16}\right) - \left(\frac{4}{3t} + \frac{1}{6}\right) = \frac{t-16}{48t}.$$

Thus, for $t > 16$, we have that for every spanning tree T of G, $R_{-1}(T) < R_{-1}(G)$.

To prove that $R_{-1}(G) \leq \frac{15(n+1)}{56}$ for connected graphs G of order $n \geq 3$, we take the same approach as done in the tree case. An inductive argument will be used. We begin with an inequality relating $R_{-1}(G)$ to $R_{-1}(G\backslash S)$. Note that deleting vertices (and edges) of G changes the degree sequence, and so the weighted graph associated with $G\backslash S$ will *not* be an induced weighted subgraph of the weighted graph associated with G.

Observation 3.3.4 *Let S be a subset of vertices of G, then,*

$$R_{-1}(G) \;\leq\; R_{-1}(G\backslash S) + \sum_{\substack{x\sim y \\ x\in S, y\notin S}} \frac{1}{d_x^G d_y^G} + \sum_{\substack{x\sim y \\ x,y\in S}} \frac{1}{d_x^G d_y^G}.$$

In [38], to prove the upper bound on $R_{-1}(T)$, the edge weights of T were summed up at the end of the proof. In general, for connected graphs it is more beneficial to use the formulation (1.7) of $R_{-1}(G)$ and sum up the vertex weights (as seen in the final case of the proof below). Some of the cases in [38, 52, 53] can be extended to general graphs, but for completeness we provide the full proof in the general case. Note that in Cases (0)-(iii) we use $1/4$ instead of $15/56$ in our manipulations of the second term. We now turn to our main result which in turn provides information about the $\mathcal{L}$-energy of connected graphs.

Theorem 3.3.5 *Let G be a connected graph on $n \geq 3$ vertices. Then*

$$R_{-1}(G) \leq \frac{15(n+1)}{56}.$$

Proof. The proof is by induction on the number of vertices. If $n = 3$, then the path of length 2 and the triangle both satisfy the inequality. Let G be a connected graph on $n \geq 4$ vertices, and assume that the inequality holds for connected graphs on fewer than n vertices.

Case (0): If G has minimum degree at least 2 then by Theorem 3.2.1, we have $R_{-1}(G) \leq n/4$, and so the inequality holds.

Case (i): Let x be a vertex of degree 1 that is adjacent to a vertex y with $d_y \geq 4$. Deleting the vertex x does not disconnect the graph, thus, using $S = \{x\}$ in Observation

3.3.4 along with induction, we have

$$\begin{aligned} R_{-1}(G) &\leq R_{-1}(G\backslash\{x\}) + \frac{1}{d_y}, \\ &\leq \frac{15}{56}n + \frac{1}{4}, \\ &< \frac{15}{56}(n+1). \end{aligned}$$

Case (ii): Let z be a vertex of degree 2 such that $z \sim x$, $z \sim y$, $d_x \leq d_y$.

(a) Suppose $x \not\sim y$ in G and either $d_x = 1, d_y \leq 2$, or $d_y \geq d_x \geq 2$. Then form a graph H by deleting z and adding the edge xy. Note that $d_x^H = d_x$ and $d_y^H = d_y$. Thus,

$$R_{-1}(G) = R_{-1}(H) + \frac{1}{2d_x} + \frac{1}{2d_y} - \frac{1}{d_x d_y}.$$

Since H has $n-1$ vertices and is connected, we have by induction that

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}n + \frac{d_x + d_y - 2}{2d_x d_y}, \\ &< \frac{15}{56}(n+1) + \frac{2d_x + 2d_y - d_x d_y - 4}{4d_x d_y}, \\ &= \frac{15}{56}(n+1) + \frac{(d_x - 2)(2 - d_y)}{4d_x d_y}. \end{aligned}$$

If $d_x = 1, d_y \leq 2$ or $d_y \geq d_x \geq 2$, then $R_{-1}(G) < \frac{15}{56}(n+1)$.

(b) Suppose $x \sim y$ in G (and hence $d_y \geq d_x \geq 2$), then

$$R_{-1}(G) \leq R_{-1}(G\backslash\{z\}) + \frac{1}{2d_x} + \frac{1}{2d_y} + \frac{1}{d_x d_y} - \frac{1}{(d_x - 1)(d_y - 1)}.$$

Since deleting z does not disconnect the graph, we have by induction that

$$R_{-1}(G) < \frac{15}{56}(n+1) - \frac{f(d_x, d_y)}{4d_x d_y (d_x - 1)(d_y - 1)},$$

where

$$f(x, y) = (x-1)(x-2)y^2 - (3x+1)(x-2)y + 2(x+2)(x-1).$$

Our goal is to show that $f(x, y) \geq 0$, for $y \geq x \geq 2$ (with x, y integral). Note that $f(2, y) = 8$, for all y. Fix $x = x_0 \geq 3$ and view f as a parabola in y opening upward. The vertex of the parabola occurs with horizontal coordinate $\frac{3}{2} + \frac{2}{x_0 - 1} \leq 2.5$. As $f(x_0, 3) = 2x_0^2 - 10x_0 + 20 \geq 0$, for $x_0 \geq 3$, we have that $f(x_0, y) \geq 0$, for $y \geq 3$. Thus, $R_{-1}(G) < \frac{15}{56}(n+1)$.

Case (iii): Assume we have vertices u, v, x, y with $d_u = 1$, $d_v = 3$, $u \sim v$, $v \sim y$, $v \sim x$ and $d_x \leq d_y$.

(a) If $d_x = 1$ and $d_y \geq 5$, then let H denote the graph obtained from G by deleting vertices x, v, and u. Note that H is a connected graph with $n - 3 \geq 3$ vertices. Thus, induction gives

$$R_{-1}(G) \leq \frac{15}{56}(n-2) + \frac{1}{3} + \frac{1}{3} + \frac{1}{15} < \frac{15}{56}(n-2) + \frac{3}{4} < \frac{15}{56}(n+1).$$

(b) Suppose $x \not\sim y$. If either: $d_x = 1, d_y \leq 4$, or $d_y \geq d_x \geq 2$, then form a new graph H obtained from G by deleting u and v and adding the edge xy. Notice that $d_x^H = d_x$ and $d_y^H = d_y$. Then

$$R_{-1}(G) = R_{-1}(H) + \frac{1}{3} + \frac{1}{3d_x} + \frac{1}{3d_y} - \frac{1}{d_x d_y}.$$

If $d_x = d_y = 1$, then G is a star on 4 vertices and the inequality holds. Otherwise, H is a connected graph with $n - 2 \geq 3$ vertices, and by induction we have

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n-1) + \frac{1}{3} + \frac{1}{3d_x} + \frac{1}{3d_y} - \frac{1}{d_x d_y}, \\ &< \frac{15}{56}(n+1) + \frac{2d_x + 2d_y - d_x d_y - 6}{6d_x d_y}, \\ &= \frac{15}{56}(n+1) + \frac{(2-d_x)d_y + 2(d_x - 3)}{6d_x d_y}. \end{aligned}$$

If $d_x = 1, d_y \leq 4$, then the numerator of the second term is nonpositive. If $d_x = 2$ or $d_x = 3$, then the the numerator of the second term is negative. If $d_y \geq d_x \geq 4$, then

$$(2 - d_x)d_y + 2(d_x - 3) \leq -2d_y + 2(d_y - 3) < 0.$$

Hence, $R_{-1}(G) < \frac{15}{56}(n+1)$ holds.

(c) Suppose $x \sim y$ and $d_y \geq d_x \geq 2$. Form a graph H by deleting u and v. Note that $d_x^H = d_x - 1$ and $d_y^H = d_y - 1$. Keeping track of the weight of edge xy in G and H gives

$$R_{-1}(G) < R_{-1}(H) + \frac{1}{3} + \frac{1}{3d_x} + \frac{1}{3d_y} + \frac{1}{d_x d_y} - \frac{1}{(d_x - 1)(d_y - 1)}.$$

Deleting u and v and using induction gives

$$R_{-1}(G) < \frac{15}{56}(n+1) - \frac{f(d_x, d_y)}{6d_x d_y (d_x - 1)(d_y - 1)},$$

where

$$f(x, y) = (x-1)(x-2)y^2 - (3x^2 - 5x - 4)y + 2(x-1)(x+3).$$

Our goal is to show that $f(x,y) \geq 0$, for $y \geq x \geq 2$ (with x, y integral). Note that $f(2,y) \geq 0$, for $y \geq 2$. Fix $x = x_0 \geq 3$ and view f as a parabola in y opening upward. The vertex occurs with horizontal coordinate $\frac{3}{2} + \frac{4x_0-10}{2(x_0-1)(x_0-2)} \leq 2$, for $x_0 = 2$ and $x_0 \geq 3$. As $f(x_0,3) = 2x_0^2 - 8x_0 + 24 \geq 0$ for $x_0 \geq 3$, we have that $f(x_0,y) \geq 0$, for $y \geq 3$. Thus, $R_{-1}(G) < \frac{15}{56}(n+1)$.

Case (iv): Let $t \geq 1$ and suppose there is a $(t, s+t)$-system of G with $s+t \geq 14$. Label the vertices as in Figure 3.1. Then deleting x_1 and y_1, and using induction gives,

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n-1) + \frac{1}{2} + \frac{1}{2d_r}, \\ &\leq \frac{15}{56}(n+1) - \frac{30}{56} + \frac{1}{2} + \frac{1}{28}, \\ &= \frac{15}{56}(n+1). \end{aligned}$$

Case (v): Suppose there is a $(t, s+t)$-system of G with $s \geq 0$ and $t \geq 4$. Label the vertices as in Figure 3.1. This system has a subgraph that is a $(4,4)$-system (that includes the vertices x_1 and y_1). By keeping track of the edge weight changes in the $(4,4)$-system subgraph and deleting x_1 and y_1, we obtain

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n-1) + \left(2 + \frac{4}{2d_r}\right) - \left(\frac{3}{2} + \frac{3}{2(d_r-1)}\right), \\ &= \frac{15}{56}(n+1) - \frac{(d_r-7)(d_r-8)}{28d_r(d_r-1)}, \\ &\leq \frac{15}{56}(n+1), \end{aligned}$$

since d_r is an integer.

Case (vi): Suppose there is a $(k, 3, s+k)$-system with $s+k \leq 14$ and $k \geq 1$. Label the vertices as in Figure 3.2. This system has a subgraph that is a $(1,3,1)$-system with center R (that includes the vertices x_1^1 and y_1^1). By keeping track of the edge weight changes in the $(1,3,1)$-system and deleting x_1^1 and y_1^1, we obtain

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n-1) + \left(\frac{3}{2} + \frac{3}{8} + \frac{1}{4d_R}\right) - \left(1 + \frac{1}{3} + \frac{1}{3d_R}\right), \\ &= \frac{15}{56}(n+1) + \frac{d_R - 14}{168d_R}, \\ &\leq \frac{15}{56}(n+1), \end{aligned}$$

since $d_R = s + k \leq 14$.

Case (vii): Suppose there is a $(k, 2, k+1)$-system of G, for some fixed $k \geq 2$. Label the vertices as in Figure 3.2. Let $u \neq r_j$, $1 \leq j \leq k$, be a vertex adjacent to R. Form a new graph H obtained from G by deleting the vertices of each $(2,3)$-system with center r_j, for $j \geq 2$, deleting R, and adding the edge ur_1. Note that the degree of u and r_1 are the same in both G and H. Then,

$$R_{-1}(G) - R_{-1}(H) = \frac{4(k-1)}{3} + \frac{k-1}{3(k+1)} + \frac{1}{3(k+1)} + \frac{1}{d_u(k+1)} - \frac{1}{3d_u}.$$

As we deleted $5(k-1)+1$ vertices to form H, we have by induction,

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n+1) - \frac{d_u(k^2-11k+44)+56(k-2)}{168d_u(k+1)}, \\ &< \frac{15}{56}(n+1), \end{aligned}$$

since $k^2 - 11k + 44 > 0$ and $k \geq 2$.

Case (viii): Let $k \geq 1$ and $t \in [1,3]$.

(a) Suppose there is a $(k, 2, k+t+1)$-system of G with center R such that R is also the center of a $(t, k+t+1)$-system (note $d_R = k+t+1$). Let u be the vertex adjacent to R that is not a vertex of one of the systems with center R. Create a new graph H by deleting the vertex R and the vertices of all the systems with center R, and adding a $(1, 2, d_u)$-system with center vertex u. A total of $5(k-1)+2t+1$ vertices have been deleted. Thus, we have by induction,

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n+1) - (5k+2t-4)\frac{15}{56} + \frac{4k}{3} + \frac{k}{3(k+t+1)} + \\ &\quad \frac{t}{2} + \frac{t}{2(k+t+1)} + \frac{1}{d_u(k+t+1)} - \frac{4}{3} - \frac{1}{3d_u}, \\ &= \frac{15}{56}(n+1) - \frac{(k^2-11k+44+6t^2+7kt-34t)d_u + 56(k+t-2)}{168d_u(k+t+1)}, \\ &< \frac{15}{56}(n+1), \end{aligned}$$

for $t \in [1,3]$ and $k \geq 1$.

(b) Suppose G has a $(k, 2, k+t)$-system with center R such that R is also the center of a $(t, k+t)$-system (note $d_R = k+t$). Then $n = 5k+2t+1$ and every vertex of G belongs

to either the $(k, 2, k+t)$-system or the $(t, k+t)$-system. Then,

$$\begin{aligned} R_{-1}(G) &= \frac{4k}{3} + \frac{k}{3(k+t)} + \frac{t}{2} + \frac{t}{2(k+t)}, \\ &= \frac{15(n+1)}{56} - \frac{k^2+7kt+34k+6t^2+6t}{168(k+t)}, \\ &< \frac{15(n+1)}{56}. \end{aligned}$$

Final Case: By Cases (i)-(iii), we may assume that every vertex of degree 1 in G is adjacent to a vertex of degree 2, and further, every vertex of degree 2 in G is adjacent to both a vertex of degree 1 and a vertex of degree at least 3. Thus, every vertex with degree 1 or 2 is contained in a system of G.

Note that if G is a (t,t)-system then $n = 2t+1$ and $R_{-1}(G) < \frac{15(n+1)}{56}$. Thus, any $(t, s+t)$-system of G (with $s \neq 1$) must have $s \geq 2$, $s+t \leq 13$ and $t \leq 3$, by Cases (iv) and (v). Any $(t, s+t)$-system with $s = 1$ belongs to a (k, t, d)-system of G.
Any $(k, t, s+k)$-system of G must have $2 \leq t \leq 3$ by Cases (ii) and (v):

- $t = 3$: For $(k, 3, d)$-systems, we must have $d \geq 15$, by Case (vi). Note that if $d = k$, then the graph is a $(k, 3, k)$-system which has $R_{-1}(G) \leq \frac{15(n+1)}{56}$.

- $t = 2$: Note that if the graph is a $(k, 2, k)$-system then $R_{-1}(G) < \frac{15}{56}(n+1)$. If G has a $(1, 2, 2)$-system, then the center of this system has degree 2 forcing G to be a $(3, 3)$-system (which has $R_{-1}(G) < \frac{15}{56}(n+1)$). Thus, for $(k, 2, s+k)$-systems, by Case (vii) we must have $s \geq 2$.

Thus, in G, the center vertex of a $(k, 2, d)$-system and $(k', 3, d)$-system may coincide, as with the center vertex of a $(k, 2, d)$-system and a (t, d)-system (but not a $(k, 3, d)$-system and (t, d)-system).

We can partition the vertices of the graph G so as to separate the systems. By Case (0), G has at least one system.

- Let A_1 be the collection of centers of $(1, d)$-systems with $3 \leq d \leq 13$ that do not share a center with any $(2, d)$-system or (k, t, d)-system.

- Let A_2 be the collection of centers of $(2, d)$-systems with $4 \leq d \leq 13$ that do not share a center with any $(3, d)$-system or (k, t, d)-system.

- Let A_3 be the collection of centers of $(3,d)$-systems with $5 \leq d \leq 13$ that do not share a center with any (k,t,d)-system.
- For $k \geq 1$, let B_k be the collection of centers of $(k,2,d)$-systems with $d \geq k+2$ that do not share a center with any $(k+1,2,d)$-system, $(k',3,d)$-system or any (i,d)-system, for $k', i \geq 1$.
- For $k \geq 1$, let C_k be the collection of centers of $(k,3,d)$-systems with $d \geq k+1$ that do not share a center with any $(k+1,3,d)$-system or $(k',2,d)$-system, for $k' \geq 1$.
- For $k_1, k_2 \geq 1$, let D_{k_1,k_2} be the collection of centers R, such that both a $(k_1,2,d)$-system and a $(k_2,3,d)$-system have center R, but R is not the center of a $(k_1+1,2,d)$-system or a $(k_2+1,3,d)$-system.
- For $i \in [1,3]$ and $k \in [1,13-i]$, let E_k^i be the collection of centers R such that both a $(k,2,d)$-system and (i,d)-system have center R, but R is not the center of a $(k+1,2,d)$-system or a $(i+1,d)$-system.

The above sets provide a partition of G into its systems. If z is the center of a system of G, then either z appears in exactly one set described above, or z is the center of a $(t,t+1)$-system that belongs to a (k,t,d)-system (whose center belongs to exactly one set described above). Let Q be the vertices of G that are have degree at least 3 and are not the center of a system of G. Then,

$$n = |Q| + 3|A_1| + 5|A_2| + 7|A_3| + \sum_{k\geq 1}(5k+1)|B_k| + \sum_{k\geq 1}(7k+1)|C_k| +$$

$$\sum_{k_1\geq 1}\sum_{k_2\geq 1}(5k_1+7k_2+1)|D_{k_1,k_2}| + \sum_{k=1}^{12}(5k+3)|E_k^1| + \sum_{k=1}^{11}(5k+5)|E_k^2| + \sum_{k=1}^{10}(5k+7)|E_k^3|.$$

By using (1.7), we will count the weight on each vertex of G. If S is a subset of vertices of G, we write $w(S)$ to denote the sum of the weights of the vertices in S.

Let $y \in Q$. Then y cannot be adjacent to degree 1 or 2 vertices, thus,

$$w(y) \leq \frac{1}{2d_y}\sum_{\substack{x\\ x\sim y}}\frac{1}{3} = \frac{1}{6} < \frac{15}{56}.$$

Let $y \in A_1$ and S_y be the set of vertices of the $(1,d_y)$-system with center y. As $d_y \geq 3$, counting the weight on the degree 1 vertex, degree 2 vertex, and y respectively, gives

$$\frac{w(S_y)}{3} \leq \frac{1}{3}\left[\frac{1}{4} + \frac{1}{4}\left(\frac{1}{d_y}+1\right) + \frac{1}{2d_y}\left(\frac{1}{2}+\frac{d_y-1}{3}\right)\right] = \frac{2d_y+1}{9d_y} < \frac{15}{56}.$$

Let $y \in A_2$ and S_y be the set of vertices of the $(2, d_y)$-system with center y. As $d_y \geq 4$,

$$\frac{w(S_y)}{5} \leq \frac{1}{5}\left[2\left(\frac{1}{4}+\frac{1}{4}\left(\frac{1}{d_y}+1\right)\right)+\frac{1}{2d_y}\left(1+\frac{d_y-2}{3}\right)\right] = \frac{7d_y+4}{30d_y} < \frac{15}{56}.$$

Let $y \in A_3$ and S_y be the set of vertices of the $(3, d_y)$-system with center y. As $d_y \geq 5$,

$$\frac{w(S_y)}{7} \leq \frac{1}{7}\left[3\left(\frac{1}{4}+\frac{1}{4}\left(\frac{1}{d_y}+1\right)\right)+\frac{1}{2d_y}\left(\frac{3}{2}+\frac{d_y-3}{3}\right)\right] = \frac{5d_y+3}{21d_y} < \frac{15}{56}.$$

Let $y \in B_k$ and S_y be the set of vertices of the $(k, 2, d_y)$-system with center y. Then

$$\frac{w(S_y)}{5k+1} \leq \frac{1}{5k+1}\left[k\left(\frac{7}{6}+\frac{1}{6}\left(1+\frac{1}{d_y}\right)\right)+\frac{1}{2d_y}\left(\frac{k}{3}+\frac{d_y-k}{3}\right)\right].$$

By subtracting $\frac{15}{56}$ from both sides, the right hand side factors as

$$\frac{w(S_y)}{5k+1}-\frac{15}{56} \leq \frac{28k-17d_y-kd_y}{168(5k+1)d_y}.$$

As $d_y \geq k+2$, we have that $28k-17d_y-kd_y \leq -(k^2-9k+34)$. When $k=4$ or $k=5$ we have $k^2-9k+34=14$. Hence, $\frac{w(S_y)}{5k+1} < \frac{15}{56}$.

Let $y \in C_k$ and S_y be the set of vertices of the $(k, 3, d_y)$-system with center y. Then,

$$\frac{w(S_y)}{7k+1} \leq \frac{1}{7k+1}\left[k\left(\frac{27}{16}+\frac{1}{8}\left(\frac{3}{2}+\frac{1}{d_y}\right)\right)+\frac{1}{2d_y}\left(\frac{k}{4}+\frac{d_y-k}{3}\right)\right].$$

By subtracting $\frac{15}{56}$ from both sides, the right hand side factors as

$$\frac{w(S_y)}{7k+1}-\frac{15}{56} \leq \frac{14k-17d_y}{168(7k+1)d_y}.$$

As $d_y \geq k$, we have that $\frac{w(S_y)}{7k+1} < \frac{15}{56}$.

Let $y \in D_{k_1,k_2}$ and S_y be the set of vertices of the $(k_1, 2, d_y)$-system and $(k_2, 3, d_y)$-system with center y. Then,

$$\frac{w(S_y)}{5k_1+7k_2+1} \leq \frac{1}{5k_1+7k_2+1}\left[k_1\left(\frac{4}{3}+\frac{1}{6d_y}\right)+k_2\left(\frac{15}{8}+\frac{1}{8d_y}\right)\right.$$
$$\left.+\frac{1}{2d_y}\left(\frac{k_1}{3}+\frac{k_2}{4}+\frac{d_y-k_1-k_2}{3}\right)\right].$$

By subtracting $\frac{15}{56}$ from both sides, the right hand side factors as

$$\frac{w(S_y)}{5k_1+7k_2+1}-\frac{15}{56} \leq -\frac{d_yk_1-28k_1-14k_2+17d_y}{168(5k_1+7k_2+1)d_y}.$$

As $d_y \geq k_1 + k_2$, we have

$$d_y k_1 - 28k_1 - 14k_2 + 17d_y \geq k_1^2 + k_1 k_2 + 3k_2 - 11k_1.$$

But $k_2 \geq 15 - k_1$, so

$$k_1^2 + k_1 k_2 + 3k_2 - 11k_1 \geq k_1 + 45 > 0.$$

Hence, $\frac{w(S_y)}{5k_1+7k_2+1} < \frac{15}{56}$.

Fix $t \in [1,3]$. Let $y \in E_k^t$ and S_y be the set of vertices of the $(k,2,d_y)$-system and (t,d_y)-system with center y. Then,

$$\frac{w(S_y)}{5k+2t+1} \leq \frac{1}{5k+2t+1}\left[k\left(\frac{4}{3}+\frac{1}{6d_y}\right)+t\left(\frac{1}{2}+\frac{1}{4d_y}\right)+\frac{1}{2d_y}\left(\frac{d_y-t}{3}+\frac{t}{2}\right)\right].$$

By subtracting $\frac{15}{56}$ from both sides, the right hand side factors as

$$\frac{w(S_y)}{5k+2t+1} - \frac{15}{56} \leq -\frac{kd_y - 28k + 6td_y - 56t + 17d_y}{168(5k+2t+1)d_y}.$$

Since $d_y = k + t + s$ with $s \geq 2$ (by Case (viii)), a simple check verifies that for $t \in [1,3]$, $k \in [1, 13-t]$ and $s \in [2, 13-t-k]$, then

$$kd_y - 28k + 6td_y - 56t + 17d_y > 0.$$

Hence, $\frac{w(S_y)}{5k+2t+1} < \frac{15}{56}$.

It now follows that $R_{-1}(G) \leq \frac{15}{56}(n+1)$, by summing the weights on each set of vertices in the partition of G. □

Observe that using $\frac{n}{4}$ instead of $\frac{15(n+1)}{56}$, then Cases (0)-(iii) in the proof of Theorem 3.3.5 hold. Thus, we can improve the upper bound in the case that G has no suspended paths.

Observation 3.3.6 *Let G be a connected graph on $n \geq 3$ vertices. If G has no suspended paths, then*

$$R_{-1}(G) \leq \frac{n}{4}.$$

3.4 The effect edge deletion has on $R_{-1}(G)$

In this section we look at the effect that edge deletion has on $R_{-1}(G)$. Recall that we call an edge $e = xy$ a *leaf* of G, if either $d_x = 1$ or $d_y = 1$, and a *non-leaf* edge otherwise. Note that deleting a leaf edge of G creates an isolated vertex, thus, in the next two results we assume the edge being deleted is a non-leaf edge. The first lemma is a result of Li and Yang.

Lemma 3.4.1 *[43, Lemma 3.3] Let G be a graph and let e be an edge whose weight is minimal over all edges in G. If e is a non-leaf edge, then*

$$R_{-1}(G-e) > R_{-1}(G).$$

In the next theorem we determine the maximum change that can occur when deleting an edge.

Theorem 3.4.2 *Let G be a graph and let e be a non-leaf edge of G, then*

$$R_{-1}(G) - \frac{1}{4} < R_{-1}(G-e) \leq R_{-1}(G) + \frac{3}{4}.$$

Furthermore, if $G-e$ is connected, then

$$R_{-1}(G-e) \leq R_{-1}(G) + \frac{7}{18}.$$

Proof. Let $e = uv$ and d_u denote d_u^G and d_v denote d_v^G. As e is a non-leaf edge, we have $d_u, d_v \geq 2$. Then

$$R_{-1}(G) - R_{-1}(G-e) = \frac{1}{d_u d_v} - \frac{1}{d_u(d_u-1)} \sum_{\substack{i \neq v \\ i \sim u}} \frac{1}{d_i} - \frac{1}{d_v(d_v-1)} \sum_{\substack{i \neq u \\ i \sim v}} \frac{1}{d_i}.$$

Thus,

$$R_{-1}(G) - R_{-1}(G-e) < \frac{1}{d_u d_v} \leq \frac{1}{4},$$

which gives the first inequality. Similarly, as $d_i \geq 1$,

$$R_{-1}(G) - R_{-1}(G-e) \;\; \geq \;\; \frac{1}{d_u d_v} - \frac{1}{d_u} - \frac{1}{d_v}.$$

It is not too hard to see that over the integers and for $d_u, d_v \geq 2$, the right hand side is minimal when $d_u = d_v = 2$. Hence,

$$R_{-1}(G) - R_{-1}(G-e) \geq \frac{-3}{4}.$$

If $G-e$ is connected, then there are vertices $\hat{i} \neq v$, $\hat{j} \neq u$ (with possibly $\hat{i} = \hat{j}$) such that $\hat{i} \sim u$, $\hat{j} \sim v$, $d_{\hat{i}} > 1$ and $d_{\hat{j}} > 1$. Thus,

$$R_{-1}(G) - R_{-1}(G-e) \geq \frac{1}{d_u d_v} - \frac{1}{2d_u(d_u-1)} - \frac{d_u-2}{d_u(d_u-1)} - \frac{1}{2d_v(d_v-1)} - \frac{d_v-2}{d_v(d_v-1)}.$$

It is not too hard to see that over the integers and for $d_u, d_v \geq 2$, the right hand side is minimal when $d_u = d_v = 3$. Hence, in the case that $G - e$ is connected,

$$R_{-1}(G) - R_{-1}(G - e) \geq \frac{-7}{18}.$$

□

We illustrate the sharpness of Theorem 3.4.2 with three examples.

Example 3.4.3 *Let G be the path on 4 vertices which has $R_{-1}(G) = 1.25$. Removing the non-leaf edge e of G, as illustrated in Figure 3.3, gives a disconnected graph with $R_{-1}(G-e) = 2$. Thus, in this case, $R_{-1}(G - e) = R_{-1}(G) + \frac{3}{4}$.*

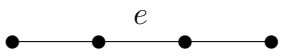

Figure 3.3: A graph G with an edge e where $R_{-1}(G - e) = R_{-1}(G) + \frac{3}{4}$.

Example 3.4.4 *Let $\hat{G}$ be the path $x_1x_2 \cdots x_7$ on 7 vertices, and add the edge $e = x_2x_6$ to form a graph G as illustrated in Figure 3.4. Then $\hat{G} = G - e$ is connected and $R_{-1}(G-e) = R_{-1}(G) + \frac{7}{18}$.*

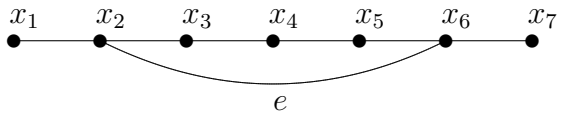

Figure 3.4: A graph G with an edge e where $R_{-1}(G - e) = R_{-1}(G) + \frac{7}{18}$.

Example 3.4.5 *Let G be the graph of order n composed of a K_{n-2} with a triangle xyz attached to a vertex z of the K_{n-2} as illustrated in Figure 3.5. Then using the edge $e = xy$, we have, $R_{-1}(G) - R_{-1}(G - e) = \frac{1}{4} - \frac{1}{n-1}$. By taking $n \to \infty$, the right hand side can be made arbitrarily close to $\frac{1}{4}$.*

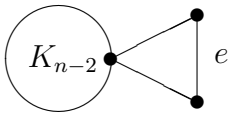

Figure 3.5: A graph G with an edge e where $R_{-1}(G) - R_{-1}(G-e) = \frac{1}{4} - \frac{1}{n-1}$.

4 THE NORMALIZED LAPLACIAN ENERGY

4.1 Introduction

Recall that the $\mathcal{L}$-*energy* of a graph G is

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{n} |\lambda_i(\mathcal{L}) - 1|.$$

In this chapter, we show

$$2 \leq E_{\mathcal{L}}(G) \leq 2 \left\lfloor \frac{n}{2} \right\rfloor,$$

and characterize the graphs attaining these bounds. If G is connected, we show that the upper bound on the $\mathcal{L}$-energy can be improved to $E_{\mathcal{L}}(G) < \sqrt{\frac{15}{28}}(n+1)$. We provide a class of connected graphs attaining $\mathcal{L}$-energy $E_{\mathcal{L}}(G) = \frac{n}{\sqrt{2}} + O(1)$ and ask if this class has maximal $\mathcal{L}$-energy over all connected graphs. Finally, we discuss other bounds for $E_{\mathcal{L}}(G)$ and how edge deletion affects $\mathcal{L}$-energy.

4.2 Upper and lower bounds on $\mathcal{L}$-energy

Using Lemma 2.7.1 along with the results in Chapter 3, bounds can be derived on the $\mathcal{L}$-energy of a graph. If G has k connected components, in particular, $G_1, G_2, \ldots, G_k$, then

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{k} E_{\mathcal{L}}(G_i). \tag{4.24}$$

We first provide a bound on the $\mathcal{L}$-energy of a graph with k connected components which is similar to the bound in Lemma 2.7.1.

Lemma 4.2.1 *Let G be a graph of order n with k connected components and no isolated vertices. Then*

$$E_{\mathcal{L}}(G) \leq k + \sqrt{(n-k)(2R_{-1}(G) - k)}.$$

Proof. Note that 1 is an eigenvalue of $I - \mathcal{L}$ with multiplicity k, hence,

$$E_{\mathcal{L}}(G) = k + \sum_{i=1}^{n-k} |\lambda_i(I - \mathcal{L})|.$$

By the Cauchy-Schwarz inequality, using vectors $(1, \ldots, 1)^T$ and

$$(|\lambda_1(I - \mathcal{L})|, \ldots, |\lambda_{n-k}(I - L)|)^T,$$

we obtain the upper bound

$$E_{\mathcal{L}}(G) \quad \leq \quad k + \sqrt{(n-k) \sum_{i=1}^{n-k} [\lambda_i(I - \mathcal{L})]^2}.$$

The result now follows by (2.21). □

We next provide bounds on the $\mathcal{L}$-energy in terms of the minimum and maximum degrees of G.

Corollary 4.2.2 *Let G be a graph of order n with k connected components and no isolated vertices. Suppose G has minimum vertex degree equal to $d_{\min}$ and maximum vertex degree equal to $d_{\max}$. Then*

$$\frac{n}{n-1} \leq \frac{n}{d_{\max}} \leq E_{\mathcal{L}}(G) \leq \frac{n}{\sqrt{d_{\min}}} \leq n.$$

Furthermore,

$$E_{\mathcal{L}}(G) \geq 2k.$$

Proof. Lemma 2.7.1 and Theorem 3.2.1 gives the first string of inequalities. For the last inequality, by (4.24), it suffices to prove $E_{\mathcal{L}}(G) \geq 2k$ in the case that $k = 1$. Note that $\lambda_n(I - \mathcal{L}) = 1$, and the trace of $I - \mathcal{L}$ is 0. Thus,

$$E_{\mathcal{L}}(G) = 1 + \sum_{i=1}^{n-1} |\lambda_i(I - \mathcal{L})| \geq 1 + \left| \sum_{i=1}^{n-1} \lambda_i(I - \mathcal{L}) \right| = 1 + |-1| = 2. \tag{4.25}$$

□

Corollary 4.2.2 implies that if G is a regular graph of degree r, then

$$\frac{n}{r} \leq E_{\mathcal{L}}(G) \leq \frac{n}{\sqrt{r}}.$$

Over the graphs of order n with no isolated vertices, we characterize those that have maximal and minimal $\mathcal{L}$-energy.

Corollary 4.2.3 *Let G be a graph of order n with no isolated vertices. Then*

$$E_{\mathcal{L}}(G) \geq 2,$$

with equality if and only if G is a complete multipartite graph. Further,

$$E_{\mathcal{L}}(G) \leq 2\lfloor n/2 \rfloor,$$

with equality if and only if G is one of the following graphs:

(i) n is even and G is the disjoint union of $n/2$ paths of length 1, or

(ii) n is odd and G is the disjoint union of $(n-3)/2$ paths of length 1 and one path of length 2, or

(iii) n is odd and G is the disjoint union of $(n-3)/2$ paths of length 1 and a complete graph on 3 vertices.

Proof. Equality in (4.25) occurs if and only if $\lambda_{n-1}(I - \mathcal{L}) \leq 0$, (equivalently $\lambda_{n-1}(A) \leq 0$). It is known that the adjacency matrix of G has only one positive eigenvalue if and only if G is a complete multipartite graph plus isolated vertices (see [17]).

(a) n is even: By Corollary 4.2.2, we have $E_{\mathcal{L}}(G) \leq n$. It can be seen that for equality to hold we must have $R_{-1}(G) = n/2$ and G must be regular of degree 1. Thus, G is the disjoint union of $n/2$ paths of length 1, which indeed has $E_{\mathcal{L}}(G) = n$.

(b) n is odd: If n is odd, we first show that for connected graphs, $E_{\mathcal{L}}(G) \leq n - 1$. If $n \geq 7$, then by Lemma 2.7.1 and Theorem 3.3.5, $E_{\mathcal{L}}(G) < n - 1$. If $n = 5$ and G has no suspended paths, then by Lemma 2.7.1 and Observation 3.3.6, $E_{\mathcal{L}}(G) < 4$. If $n = 5$ and has a suspended path, then there are only three such graphs and each has $E_{\mathcal{L}}(G) < 4$. If $n = 3$, then both the path of length 2 and the complete graph on 3 vertices have energy $n - 1 = 2$. This implies that if n is odd and G is a connected graph of order n, then $E_{\mathcal{L}}(G) \leq n - 1$. Equality in this bound occurs if and only if $n = 3$ and either G is a path of length 2 or a complete graph K_3.

Now suppose that G has $k \geq 2$ connected components, in particular,

$$G_1, G_2, \ldots, G_k,$$

with each component G_i having n_i vertices. Without loss of generality, suppose that $n_1, \ldots, n_s$ are odd and $n_{s+1}, \ldots, n_k$ are even. Since n is odd, $s \geq 1$. By (4.24),

$$\begin{aligned} E_{\mathcal{L}}(G) &= \sum_{i=1}^{s} E_{\mathcal{L}}(G_i) + \sum_{i=s+1}^{n} E_{\mathcal{L}}(G_i), \\ &\leq \sum_{i=1}^{s} (n_i - 1) + \sum_{i=s+1}^{n} n_i, \\ &= n - s, \\ &\leq n - 1. \end{aligned}$$

For equality $E_{\mathcal{L}}(G) = n - 1$ to hold, G can have only one odd connected component which, by the above, must be of order 3. Any even connected component must be a path of length 1, thus G must be one of the graphs listed in (ii) or (iii). Since the graphs in (ii) and (iii) have energy $n - 1$, this completes the proof. □

4.3 Bounds on $\mathcal{L}$-energy over the class of connected graphs

The upper bound in Corollary 4.2.3 can be improved for connected graphs by using Lemma 2.7.1 and Theorem 3.3.5.

Corollary 4.3.1 *If G is a connected graph on $n \geq 3$ vertices, then*

$$E_{\mathcal{L}}(G) < \sqrt{\frac{15}{28}}(n+1) < 0.732(n+1).$$

Furthermore, if G has no suspended paths (or more generally, $R_{-1}(G) \leq \frac{n}{4}$), then

$$E_{\mathcal{L}}(G) \leq \frac{n}{\sqrt{2}} < 0.7072\ n.$$

One might suspect that over the connected graphs that the path has maximal $\mathcal{L}$-energy, but in general, this is not true. We next provide some classes of graphs along with their corresponding $\mathcal{L}$-energy.

Example 4.3.2 *Let G be a path on n vertices. Using the eigenvalues of $\mathcal{L}$ (see Example 1.6.3) we obtain*

$$E_{\mathcal{L}}(G) = 2 \sum_{k=0}^{\lfloor (n-1)/2 \rfloor} \cos(k\pi/(n-1)).$$

By [28, page 37],

$$\sum_{k=0}^{N} \cos(kx) = \cos\left(\frac{Nx}{2}\right) \sin\left(\frac{N+1}{2}x\right) \csc\left(\frac{x}{2}\right).$$

Thus, for the path, $E_{\mathcal{L}}(G) \sim \frac{2}{\pi}n$.

Example 4.3.3 *(a) For* n *odd, let* G *be a* (t,t)*-system with* $n = 2t+1$ *vertices. The normalized Laplacian matrix of* G *can be written in block form as*

$$\mathcal{L} = \begin{bmatrix} I_t & -\frac{1}{\sqrt{2}}I_t & \mathbf{0}_t \\ -\frac{1}{\sqrt{2}}I_t & I_t & -\frac{1}{\sqrt{2t}}\mathbf{1}_t \\ \mathbf{0}_t^T & -\frac{1}{\sqrt{2t}}\mathbf{1}_t^T & 1 \end{bmatrix}.$$

Thus, the eigenvalues are 0, 1, 2, *each with multiplicity* 1, *and* $(1 \pm \frac{1}{\sqrt{2}})$ *each with multiplicity* $t-1$. *Hence, the* $\mathcal{L}$*-energy is*

$$E_{\mathcal{L}}(G) = \frac{n-3}{\sqrt{2}} + 2 \sim \frac{n}{\sqrt{2}}.$$

(b) For $n = 2t+2$ *even, let* G *be the graph obtained by joining a vertex to a leaf of a* (t,t)*-system. The normalized Laplacian matrix of* G *can be written in block form as*

$$\mathcal{L} = \begin{bmatrix} 1 & -\frac{1}{\sqrt{2}} & \mathbf{0}_{t-1}^T & 0 & \mathbf{0}_{t-1}^T & 0 \\ -\frac{1}{\sqrt{2}} & 1 & \mathbf{0}_{t-1}^T & -\frac{1}{2} & \mathbf{0}_{t-1}^T & 0 \\ \mathbf{0}_{t-1} & \mathbf{0}_{t-1} & I_{t-1} & \mathbf{0}_{t-1} & -\frac{1}{\sqrt{2}}I_{t-1} & \mathbf{0}_{t-1} \\ 0 & -\frac{1}{2} & \mathbf{0}_{t-1}^T & 1 & \mathbf{0}_{t-1}^T & -\frac{1}{\sqrt{2t}} \\ \mathbf{0}_{t-1} & \mathbf{0}_{t-1} & -\frac{1}{\sqrt{2}}I_{t-1} & \mathbf{0}_{t-1} & I_{t-1} & -\frac{1}{\sqrt{2t}}\mathbf{1}_{t-1} \\ 0 & 0 & \mathbf{0}_{t-1}^T & -\frac{1}{\sqrt{2t}} & -\frac{1}{\sqrt{2t}}\mathbf{1}_{t-1}^T & 1 \end{bmatrix}.$$

The eigenvalues of this matrix are 0 *and* 2 *each with multiplicity* 1, $(1 \pm \frac{1}{\sqrt{2}})$ *each with multiplicity* $t-2$ *along with four other eigenvalues. To find the four missing eigenvalues we use the fact that each block of* $\mathcal{L}$ *has constant row sums thus forming an equitable partition. The quotient matrix is*

$$\begin{bmatrix} 1 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ -\frac{1}{\sqrt{2}} & 1 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 & -\frac{1}{\sqrt{2}} & 0 \\ 0 & -\frac{1}{2} & 0 & 1 & 0 & -\frac{1}{\sqrt{2t}} \\ 0 & 0 & -\frac{1}{\sqrt{2}} & 0 & 1 & -\frac{1}{\sqrt{2t}} \\ 0 & 0 & 0 & -\frac{1}{\sqrt{2t}} & -\frac{(t-1)}{\sqrt{2t}} & 1 \end{bmatrix}.$$

Thus, the four missing eigenvalues are:

$$1 \pm \frac{\sqrt{6t^2 \pm 2t\sqrt{9t^2-8t}}}{4t},$$

each with multiplicity 1. *Note that as* $t \to \infty$, *these four eigenvalues approach* $1, 1, 1 \pm \frac{\sqrt{3}}{2}$. *This implies that*

$$E_{\mathcal{L}}(G) \sim \frac{n}{\sqrt{2}}.$$

Example 4.3.3 provides a class of graphs with $\mathcal{L}$-energy asymptotic to $\frac{n}{\sqrt{2}}$ and $R_{-1}(G)$ asymptotic to $\frac{n}{4}$. However, there is a small gap between the $\mathcal{L}$-energy of the graphs in Example 4.3.3 and the first bound listed in Corollary 4.3.1. In order to find graphs with $\mathcal{L}$-energy asymptotically larger than $\frac{n}{\sqrt{2}}$ we might consider graphs that have $R_{-1}(G)$ asymptotically larger than $\frac{n}{4}$. In particular, a $(t,3,t)$-system (with $n = 7t+1$ vertices) and a $(t,2,t)$-system (with $n = 5t+1$ vertices) have $R_{-1}(G)$ asymptotic to $\frac{15}{56}n$ and $\frac{4}{15}n$ respectively. If G is a $(t,3,t)$-system with $n = 7t+1$, then using a computer to test large values of n suggests that $E_{\mathcal{L}}(G) \approx 0.671n$. Similarly, if G is a $(t,2,t)$-system with $n = 5t+1$, then using a computer to test large values of n suggests that $E_{\mathcal{L}}(G) \approx 0.648n$. It is curious that the $\mathcal{L}$-energies of these two systems are much smaller than $\frac{n}{\sqrt{2}}$, yet their respective general Randić indices are larger than that of Example 4.3.3.

For small values of n, Matlab was used to find maximal $\mathcal{L}$-energy connected graphs for $3 \leq n \leq 10$ by using a database of nonisomorphic connected graphs (in particular, [48]). For $n = 3$, the path and triangle each have maximal $\mathcal{L}$-energy of 2. For $4 \leq n \leq 6$, the path has maximal $\mathcal{L}$-energy over the class of connected graphs. Note that for $4 \leq n \leq 6$, the path falls under the class of graphs described in Example 4.3.3. For $7 \leq n \leq 10$, over all connected graphs, the class of graphs in Example 4.3.3 have maximal $\mathcal{L}$-energy. For $n \geq 11$, it is unknown which connected graphs have maximal $\mathcal{L}$-energy.

We know of no class of connected graphs on n vertices that has $\mathcal{L}$-energy (asymptotically) larger than $\frac{n}{\sqrt{2}}$. Corollary 4.3.1 implies such a graph G would have $R_{-1}(G) > \frac{n}{4}$ and Observation 3.3.6 suggests such a graph should have a large number of suspended paths. Based on our discussion above regarding the $\mathcal{L}$-energy of a $(t,3,t)$-system and a $(t,2,t)$-system, we ask the question: Over the connected graphs G of order n, is $E_{\mathcal{L}}(G) \leq \frac{n}{\sqrt{2}} + C$, for some suitable constant C? We put forth the following conjecture.

Conjecture 4.3.4 *The graphs in Example 4.3.3 have maximal* $\mathcal{L}$*-energy over the class of connected graphs on* n *vertices.*

4.4 Other bounds on $\mathcal{L}$-energy

We now look at other bounds on $\mathcal{L}$-energy. We start with a lower bound that uses the arithmetic-geometric mean inequality.

Theorem 4.4.1 *Let G be a graph of order n with no isolated vertices and let $\Delta = \det(I-\mathcal{L})$. Then*

$$E_{\mathcal{L}}(G) \geq \sqrt{2R_{-1}(G) + n(n-1)\Delta^{2/n}}.$$

Proof. Note that

$$\begin{aligned} E_{\mathcal{L}}(G)^2 &= \sum_{i=1}^{n} |1-\lambda_i(\mathcal{L})|^2 + 2\sum_{1\leq i<j\leq n} |1-\lambda_i(\mathcal{L})||1-\lambda_j(\mathcal{L})|, \\ &= 2R_{-1}(G) + \sum_{i\neq j} |1-\lambda_i(\mathcal{L})||1-\lambda_j(\mathcal{L})|. \end{aligned}$$

By the arithmetic-geometric mean inequality,

$$\frac{1}{n(n-1)}\sum_{i\neq j} |1-\lambda_i(\mathcal{L})||1-\lambda_j(\mathcal{L})| \geq \left(\prod_{i\neq j} |1-\lambda_i(\mathcal{L})||1-\lambda_j(\mathcal{L})|\right)^{\frac{1}{n(n-1)}} = \Delta^{2/n}.$$

Hence, the result now follows. □

We next relate the $\mathcal{L}$-energy of a graph G to its A-energy, where A is the adjacency matrix of G. Recall that the A-energy is simply

$$E_A(G) = \sum_{i=1}^{n} |\lambda_i(A)|.$$

This quantity has been well studied by a large number of authors (see, for example, [30]). The following result follows readily from Theorem 2.2.1.

Corollary 4.4.2 *Let G be a graph of order n with no isolated vertices. Suppose $d_{\min}$ and $d_{\max}$ are the minimum and maximum vertex degrees of G, respectively. Then,*

$$d_{\min}E_{\mathcal{L}}(G) \leq E_A(G) \leq d_{\max}E_{\mathcal{L}}(G).$$

Corollary 4.4.2 implies that if G is a regular graph of degree r, then $E_A(G) = rE_{\mathcal{L}}(G)$. Since $E_A(G)$ is well studied, many bounds for $E_A(G)$ in the literature can be applied to $E_{\mathcal{L}}(G)$ by way of Corollary 4.4.2.

4.5 The effect edge deletion has on $\mathcal{L}$-energy

In this section, we look at the effect edge deletion has on $E_{\mathcal{L}}(G)$. We begin with examples to show that $\mathcal{L}$-energy can increase, decrease or remain unchanged upon edge deletion. The examples will also illustrate that the effect edge deletion has on the general Randić index does not necessarily provide direct information about the effect edge deletion has on $\mathcal{L}$-energy.

Example 4.5.1 *In this example, we list the $\mathcal{L}$-energy and general Randić index (to three decimal places if appropriate) for each graph in Figures 4.1, 4.2 and 4.3.*

(i) The graphs in Figure 4.1 have a decrease in $\mathcal{L}$-energy upon deleting edge e. For the first (resp. second and third) graph, $2 = E_{\mathcal{L}}(G-e) < E_{\mathcal{L}}(G) \approx 2.457$ (resp. $2 = E_{\mathcal{L}}(G-e) < E_{\mathcal{L}}(G) \approx 2.618$ and $2 = E_{\mathcal{L}}(G-e) < E_{\mathcal{L}}(G) \approx 2.704$). For the first (resp. second and third) graph, $1 = R_{-1}(G-e) > R_{-1}(G) \approx 0.917$ (resp. $R_{-1}(G-e) = R_{-1}(G) = 1$ and $1 = R_{-1}(G-e) < R_{-1}(G) = 1.05$).

(ii) The graphs in Figure 4.2 have an increase in $\mathcal{L}$-energy upon deleting edge e. For the first (resp. second and third) graph, $2.869 \approx E_{\mathcal{L}}(G-e) > E_{\mathcal{L}}(G) \approx 2.667$ (resp. $3.076 \approx E_{\mathcal{L}}(G-e) > E_{\mathcal{L}}(G) \approx 2.904$ and $3.117 \approx E_{\mathcal{L}}(G-e) > E_{\mathcal{L}}(G) = 3$). For the first (resp. second and third) graph, $1.111 \approx R_{-1}(G-e) > R_{-1}(G) \approx 1.028$ (resp. $R_{-1}(G-e) = R_{-1}(G) \approx 1.007$ and $0.928 \approx R_{-1}(G-e) < R_{-1}(G) \approx 0.978$).

(iii) The graphs in Figure 4.3 have no change in $\mathcal{L}$-energy upon deleting edge e. For the first (resp. second) graph, $E_{\mathcal{L}}(G-e) = E_{\mathcal{L}}(G) = 2$ (resp. $E_{\mathcal{L}}(G-e) = E_{\mathcal{L}}(G) \approx 2.781$). For the first (resp. second) graph, $1 = R_{-1}(G-e) > R_{-1}(G) = 0.75$ (resp. $R_{-1}(G-e) = R_{-1}(G) = 1.0625$). The only remaining case is where upon edge deletion, $\mathcal{L}$-energy remains constant while $R_{-1}(G)$ decreases. We do not know of a graph that has this property.

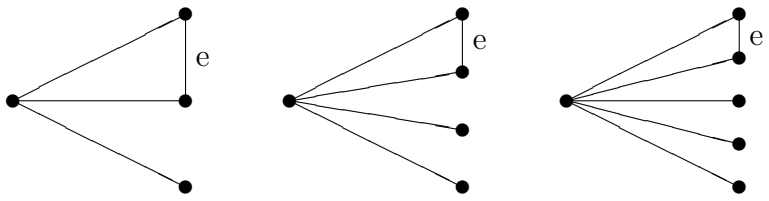

Figure 4.1: Graphs for which $\mathcal{L}$-energy decreases upon deleting edge e.

The next result provides a bound on how much the $\mathcal{L}$-energy can change upon edge deletion.

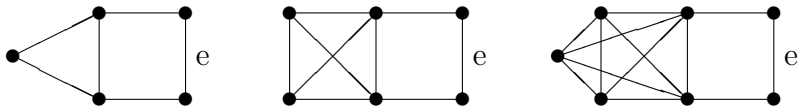

Figure 4.2: Graphs for which $\mathcal{L}$-energy increases upon deleting edge e.

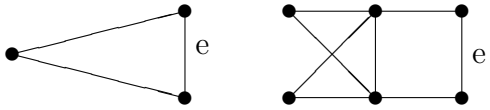

Figure 4.3: Graphs for which $\mathcal{L}$-energy remains constant upon deleting edge e.

Theorem 4.5.2 *Let G be a graph of order n without isolated vertices and let e be a non-leaf edge of G. Then,*

$$|E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G-e)| \leq 2\sqrt{\frac{13}{2} - 4\sqrt{2}} \leq 1.8366.$$

Proof. Let $\mathcal{L}_G$ and $\mathcal{L}_{G-e}$ be the normalized Laplacian matrices of G and $G-e$, and suppose $e = xy$. Let $C = \mathcal{L}_G - \mathcal{L}_{G-e}$. Observe that by Theorem 1.4.2, we can derive

$$|E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G-e)| \leq \sum_{i=1}^{n} \sigma_i(C).$$

Note that $rank(C) \leq 4$. Let the eigenvalues of C be 0 with multiplicity $n-4$ and $\lambda_1, \lambda_2, \lambda_3, \lambda_4$.Then,

$$\sum_{i=1}^{n} \sigma_i(C) = |\lambda_1| + |\lambda_2| + |\lambda_3| + |\lambda_4|.$$

By the Cauchy-Schwarz inequality, $|E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G-e)| \leq 2\sqrt{tr(C^2)}$, which equals:

$$2\sqrt{2}\sqrt{\frac{1}{d_x d_y} + \sum_{\substack{j\neq y \\ j\sim x}} \left(\frac{1}{\sqrt{d_x d_j}} - \frac{1}{\sqrt{(d_x-1)d_j}}\right)^2 + \sum_{\substack{j\neq x \\ j\sim y}} \left(\frac{1}{\sqrt{d_y d_j}} - \frac{1}{\sqrt{(d_y-1)d_j}}\right)^2},$$

$$\leq 2\sqrt{2}\sqrt{\frac{1}{4} + \frac{\left(\sqrt{d_x - 1} - \sqrt{d_x}\right)^2}{d_x} + \frac{\left(\sqrt{d_y - 1} - \sqrt{d_y}\right)^2}{d_y}}.$$

The $\frac{1}{4}$ comes from setting $d_x = d_y = 2$, as this is when the first term is maximal, and the other two expressions come from noticing $d_j \geq 1$. The function

$$f(x) = \frac{\left(\sqrt{x-1} - \sqrt{x}\right)^2}{x}$$

has $f'(x) < 0$, for $x > 1$. Thus, as $d_x, d_y \geq 2$, $|E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G - e)| \leq 2\sqrt{\frac{13}{2} - 4\sqrt{2}}$. □

5 SUMMARY AND FUTURE CONSIDERATIONS

5.1 Largest normalized Laplacian eigenvalue

In [12], there is a great emphasis on finding bounds on $\lambda_2(\mathcal{L})$ and its relationship to the Cheeger constant. However, there is not much discussed in [12] regarding bounds on $\lambda_n(\mathcal{L})$. As discussed in Section 2.4, an intuitive interpretation of $\lambda_n(\mathcal{L})$ is a measure of how close a graph is to being bipartite. It would be interesting to determine bounds on $\lambda_n(\mathcal{L})$ in terms of other parameters of a graph, for example, the diameter. Note that Chung does make a connection between diamater, $\lambda_2(\mathcal{L})$ and $\lambda_n(\mathcal{L})$ (for example, see [12, Equation 3.2]). Other bounds could be obtained by extending results from the recent paper by Trevisan [64], where the concept of the bipartiteness ratio of a graph is introduced and bounded in terms of $\lambda_1(\frac{1}{r}A)$ for r-regular graphs.

One reason to analyze $\lambda_n(\mathcal{L})$ in more detail is because $\max_{i\neq 1}|1-\lambda_i(\mathcal{L})|$ shows up when looking at random walks, and the maximum occurs at either $\lambda_2(\mathcal{L})$ or $\lambda_n(\mathcal{L})$. Chung claims that when analyzing random walks in weighted graphs only $\lambda_2(\mathcal{L})$ is crucial in the sense that if $\lambda_n(\mathcal{L})-1 \geq 1-\lambda_2(\mathcal{L})$ then one can form a new graph G' by adding loops and consider a modified random walk called the lazy walk. Then, in the new graph, the upper bound for the distance between the stationary distribution and the k-step distribution can be written in terms of $\lambda_2(\mathcal{L})$ while omitting $\lambda_n(\mathcal{L})$. However, when dealing with random walks on simple undirected graphs, $\lambda_n(\mathcal{L})$ does play an important role. A more indepth study of $\lambda_n(\mathcal{L})$ is needed given its importance when looking at the structure of a graph and its relationship to random walks.

5.2 Cospectral graphs with respect to the $\mathcal{L}$-eigenvalues

It should be noted that if G_1 and G_2 are both complete bipartite graphs on the same number of vertices, then they are cospectral with respect to the $\mathcal{L}$-eigenvalues. This demonstrates that cospectral graphs with respect to $\mathcal{L}$ do not require the same number of edges. This is contrary to being cospectral with respect to the adjacency eigenvalues.

An interesting example of cospectral graphs with respect to the $\mathcal{L}$-eigenvalues is the following. Let G be the graph on the right in Figure 4.3 and e the labelled edge. It was mentioned that G and $G - e$ have the same $\mathcal{L}$-energy. In fact, a stronger statement holds, that is, G and $G - e$ are cospectral with respect to the $\mathcal{L}$-eigenvalues. In this case, edge deletion does not change the $\mathcal{L}$-spectrum. It is interesting to know if other graphs exist with the property that edge deletion does not change the $\mathcal{L}$-spectrum.

5.3 Graphs having exactly three distinct $\mathcal{L}$-eigenvalues

We know of no graph that has exactly three distinct $\mathcal{L}$-eigenvalues and at least four distinct vertex degrees. If such a graph does not exist, perhaps (2.14) can be used to show this. Further, Theorem 2.6.6 provides graphs with three distinct vertex degrees that have a vertex of degree 1. We ask the question if there exists graphs with three distinct $\mathcal{L}$ eigenvalues and three distinct vertex degrees such that no vertex is of degree 1.

It would be interesting to know in the case of a graph G with exactly three distinct $\mathcal{L}$-eigenvalues and two distinct vertex degrees (partitioned into parts $A \cup B$, where vertices in A have the same degree and vertices in B have the same degree), if the induced subgraph of G on A and the induced subgraph of G on B need to be a strongly regular graph, the complete graph, or the empty graph. If so, a technique similar to that of the proof of Theorem 2.6.6 might work.

5.4 The general Randić index $R_{-1}(G)$

Since the motivation for the general Randić index originated from theoretical chemistry, many of the older results that are known about $R_\alpha(G)$ are for trees. Recently, there has been some interest in $R_\alpha(G)$ for general graphs.

The strong connection between $R_{-1}(G)$ and the normalized Laplacian spectrum provides motivation to study the behaviour of $R_{-1}(G)$ for graphs in general and not just trees. A first

step would be to refine the bound in Theorem 3.3.5, that is, provide a sharp upper bound for all values of n. Given the corresponding result for trees (of order $n \geq 720$), this will definitely take some careful consideration. In particular, Pavlović, Stojanović and Li [53] proved the following for trees.

Theorem 5.4.1 *[53] For a tree T_n^t of order $n \geq 720$,*

$$R_{-1}(T_n^T) \leq R_{-1}^*(T_n^t) = \begin{cases} \frac{15n-1}{56}, & t = 0 \\ \frac{15n-1}{56} - \frac{1}{56} + \frac{7}{4(n+5)}, & t = 1 \\ \frac{15n-1}{56} - \frac{3}{5} \cdot \frac{1}{56} - \frac{7}{20(n-3)}, & t = 2 \\ \frac{15n-1}{56} - \frac{2}{3} \cdot \frac{1}{56} + \frac{7}{6(n+3)}, & t = 3 \\ \frac{15n-1}{56} - \frac{6}{5} \cdot \frac{1}{56} - \frac{7}{20(n-12)}, & t = 4 \\ \frac{15n-1}{56} - \frac{1}{3} \cdot \frac{1}{56} + \frac{7}{12(n+1)}, & t = 5 \\ \frac{15n-1}{56} - \frac{29}{27} \cdot \frac{1}{56} - \frac{35}{36(n-35)}, & t = 6, \end{cases}$$

where $R_{-1}^*(T_n^t)$ is the maximum value of the general Randić index over the class of trees of order n with n congruent to t (modulo 7).

Pavlović, Stojanović and Li [53] also provided classes of trees of every order n (with $n \geq 720$) that achieves the maximum value in Theorem 5.4.1. We suspect a similar result holds for $R_{-1}(G)$ over the class of connected graphs, perhaps with the same maximum values as in the tree case. One approach is to show that for each n, there is a tree on n vertices that maximizes $R_{-1}(G)$ over the connected graphs of order n. As demonstrated in Example 3.3.3, looking at the spanning trees is not enough.

5.5 Normalized Laplacian energy

Settling Conjecture 4.3.4 is an open problem. A lot of evidence has been provided to demonstrate why Conjecture 4.3.4 may be true and perhaps a more detailed look at the general Randić index and its relationship to the $\mathcal{L}$-eigenvalues will help.

The bound given in Theorem 4.5.2 on the maximum change in $\mathcal{L}$-energy when an edge is deleted is far from optimal. Matlab suggests that using the method in the proof of Theorem 4.5.2 can do no better than 1.56 as an upper bound on $|E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G - e)|$. If we have additional information about the graph, then analyzing the inequalities in the proof can improve the bound. In particular, if we have vertices with large degree, then the upper

bound becomes much smaller. Thus, a technique to handle vertices of low degree can be combined with the proof of Theorem 4.5.2 to obtain a refined upper bound. It should be noted that before using the singular value approach in Theorem 4.5.2 that an interlacing technique was attempted (in the obvious manner), however, this produced weaker bounds of $-4 \leq E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G-e) \leq 2$. We ask, what are the optimal values of c_1 and c_2 so that

$$-c_1 \leq E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G-e) \leq c_2$$

holds for any graph G and edge e of G (where G and $G-e$ contain no isolated vertices). Theorem 4.5.2 shows that $c_1, c_2 \leq 1.8366$ and examples of graphs are known that show $c_1 \geq 1$ and $c_2 \geq 0.7575$. We suspect that $c_1 = 1$ is optimal and that $c_2 < 1$, however, determining the true values of c_1, c_2 remains an open problem.

The analagous problem for energy (allowing graphs with isolated vertices) has been solved as illustrated in the following result due to Day and So.

Lemma 5.5.1 *[22, Corollary 2.7] Let e be an edge of a graph G, then*

$$-2 \leq E_A(G) - E_A(G-e) \leq 2.$$

Equality in the upper bound holds if and only if e is an isolated edge of G and equality in the lower bound never holds.

Furthermore, an example provided by S. Cioabă (see [22, Example 3.5]) shows that the gap in the lower bound in Lemma 5.5.1 can be arbitrarily small.

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