On the k-Independence Number and Laplacian Toughness of Graphs

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Abstract

Eigenvalue interlacing and quotient matrices are crucial tools in algebraic graph theory, essential for analyzing and proving bounds for critical graph parameters. This work focuses on themes of independence number, connectivity, graph toughness, and closed walks in infinite regular trees.

Computing the k-independence number of a graph, which is the size of a largest set of vertices that are a distance greater than k apart in the graph, is NP-complete. In other words there is no known algorithm that can find the k-independence number of a graph in a polynomial time. So bounds are important to analyse this parameter in graphs. This thesis is based on an algebraic approach which requires identifying a polynomial in order to get a good bound. Optimal polynomials have been found by other authors for the values $k = 1, 2$. In our work, we proved the optimal polynomial for $k = 3$ and thus determining the 3-independence number for several families of graphs. For instance, we proved bounds for the Hamming graphs, which are tight for some families. We also give a construction of 3-independent sets in the Hamming graph $H(d, 2)$, also known as Hypercubes. Hamming graphs play an important role in coding theory. Codes and anticodes are k-independent sets in the Hamming graph, so our bounds constrain possible codes.

Solving for these optimal polynomials require our knowledge of the number of closed walks centered on the vertices of the graph. This leads to an exploration of the number of closed walks in an infinite d-regular tree that start and end at a vertex. In the second theme of this thesis, we count closed walks in an infinite regular tree using Catalan's triangle and Borel's triangle. Specifically, we demonstrate that the number of closed walks centered on a vertex forms a polynomial in d, with coefficients aligning with the terms of the Borel triangle. These arrays of numbers, with diverse applications in mathematics, offer alternative perspectives on the underlying combinatorial structures.

Turning our attention to connectivity and toughness, we present an improved bound on vertex connectivity initially proposed by Krivelevich and Sudakov. An intimately connected concept is graph toughness, which quantifies how closely various parts of a graph are interconnected. This concept was introduced by Chvatal in 1973 and has since spurred significant research, much of it stemming from conjectures in his seminal paper. Graph toughness is linked to numerous graph properties, including

Hamiltonicity, connectivity, spanning trees, graph factors, and more. In this thesis, we derived bounds on graph toughness and establish cases of a Laplacian bound on graph toughness conjectured by Haemers. Specifically, we confirm the conjecture for regular bipartite graphs, trees, and graphs with at least one leaf. We also establish the conjecture for graphs on up to 8 vertices, and some particular constructed graphs.

Dedication

To my sweethearts Rhoda, Yesutor, Elikplim, and Seyram, who bore the sharp brunts of student life.

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"To the end that my glory may sing praise to thee, and not be silent. O LORD my God, I will give thanks unto thee for ever." – Psalm 30:12

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Chapter 1

Introduction

Eigenvalue interlacing and quotient matrices are fundamental tools in algebraic graph theory, playing a pivotal role in the study and proof of bounds for critical graph properties. These properties encompass the size of a maximal clique, the size of a maximal independent set, the chromatic number, the diameter, and more, all through the spectrum of the adjacency matrix or Laplacian matrix of a graph. Notable surveys of this topic can be found in Haemers' papers [39, 41, 42], with additional insights relevant to this thesis provided by Fiol's work [30].

In this thesis, we delve into closely related themes, including independence number, connectivity, and graph toughness. Additionally, we present combinatorial results concerning the number of closed walks in infinite regular trees.

An independent set, also known as a stable set or coclique, in a graph is a set of vertices where no two are adjacent. The size of the largest independent set is termed the independence number. Two classical eigenvalue bounds on the independence number, proved using interlacing (though also established via other techniques [43]), are Hoffman's ratio bound [42] and Cvetković's inertia bound [23]. Of particular interest to us is the concept of a k-independent set, where any two vertices in the set are at distance at least $k+1$ from each other in the graph. There are other uses of this term in the literature, see [16, 65]. The k-independence number, denoted as α_k, represents the size of the largest k-independent set. Using interlacing, Abiad et al. [1, 2] extended the Hoffman and Cvetković spectral bounds to k-independence, involving polynomials of degree at most k. Selecting the right polynomial is crucial for obtaining a good bound. The bound obtained from the polynomial does not change if the polynomial is scaled or shifted so we may assume the polynomial is monic and has no constant term. For the generalized Hoffman bound for α_k, the polynomial $p(x) = x$ gives the standard Hoffman bound for the independence number α_1. The authors of [2] gave the optimal polynomial for $k = 2$, and proposed a polynomial for a general $k \geq 3$ though it may not be the best choice in general. Fiol [31] also introduced the so called minor polynomials for this purpose.

In our current work, we determine the optimal polynomial to bound the 3-independence number. We explore the polynomial $p(x) = x^3 + bx^2 + cx$, where b and c are real numbers. For a fixed b, we identify the eigenvalue that minimizes $p(x)$ within a specified interval for c. This analysis is detailed in Lemma 4.2.1. With this polynomial, we derive an upper bound on the 3-independence number as

$$n\frac{\triangle - \theta_0(\theta_s + \theta_{s+1} + \theta_d) - \theta_s\theta_{s+1}\theta_d}{(\theta_0 - \theta_s)(\theta_0 - \theta_{s+1})(\theta_0 - \theta_d)}$$

where θ_s is a specified eigenvalue of the graph and $\triangle$ is twice the largest number of triangles centred on a vertex in the graph. These findings are encapsulated in Theorem 4.2.2. This and related results appear in [49]. We present 3-independence bounds on various graph families, including the Hamming graph and the Johnson graph, demonstrating tightness in several instances. Through our analysis, we identified common patterns that suggest a general form for the optimal polynomial for any value of k.

The k-independence number has implications for various graph properties, including average distance [32], packing chromatic number [33], injective chromatic number [44], and strong chromatic index [57], as highlighted in [1, 31]. Upper bounds on the k-independence number translate to lower bounds on related properties, such as distance and packing chromatic numbers [1]. The k-independence number is also related to coding theory (for instance, codes and anticodes are k-independent sets in the Hamming graph [56]).

The technique we employ in solving the k-independence number of a graph requires knowledge of the number of closed walks centered on the vertices. For $k > 3$, determining this number becomes challenging, prompting us to explore graphs with large girth, ideally of size $k + 1$ or greater. When localized to a vertex, such graphs resemble regular trees. A finite regular graph with girth greater than $2n$ effectively acts as a tree locally, allowing us to apply results on the number of closed walks from infinite regular trees. In Chapter 6, we delve into the exploration of closed walks on vertices in an infinite δ-regular tree G. Specifically, we investigate the number of closed walks of length $2n$ centered on a vertex. Traditionally, enumerating closed walks on a vertex in a regular tree has been approached through generating functions. However, in this thesis, we introduce a combinatorial method for counting closed walks using Catalan's triangle and Borel's triangle. These arrays of numbers, with diverse applications in mathematics, offer alternative perspectives on the underlying combinatorial structures. The major results in Chapter 6 are Theorem 6.3.8, which provides a formula in terms of Catalan numbers, and Theorem 6.3.11, which offers a formula in terms of the numbers in Borel's triangles. In particular, we establish that the number of closed walks centered on a vertex can be expressed as a polynomial in δ, where the coefficients correspond to the terms of the Borel triangle.

Turning our attention to connectivity and toughness, we present an improved bound on vertex connectivity initially proposed by Krivelevich and Sudakov [50]. An intimately connected concept is graph toughness, which quantifies how closely various parts of a graph are interconnected. This concept was introduced by Chvátal in 1973 and has since spurred significant research, much of it stemming from conjectures in his seminal paper [19]. Graph toughness is linked to numerous graph properties, including Hamiltonicity, connectivity, spanning trees, graph factors, and more. A k-factor of a graph is a k-regular spanning subgraph. In this thesis, we derive bounds on graph toughness and establish cases of a Laplacian bound on graph toughness conjectured by Haemers [40]. Specifically, we confirm the conjecture for regular bipartite graphs, trees, and graphs with at least one leaf. We also establish the conjecture for some particular graphs.

This thesis is organized into chapters as follows:

- In Chapter 2, we provide essential background information to facilitate an understanding of the subsequent chapters.
- In Chapter 3, we introduce the two classical algebraic bounds on the independence number and describe their generalization to the k-independence number in [1, 2].
- Chapter 4 presents the optimal bound on the 3-independence number.
- In Chapter 5, we explore the applications of the 3-independence number on specific classes of graphs. We derive bounds and provide constructions of 3-independence sets in the Hamming graph. We also propose an optimal polynomial for any k.
- In Chapter 6, we count the number of closed walks in a regular tree using Catalan and Borel's triangles.
- Chapter 7 delves into our work on the connectivity and toughness of graphs. This chapter also contains the background and some previous works done on spectral bounds on graph toughness.

Chapters 4 and 5 were published as the article [49] while the material from Chapter 6 can be found in the preprint [48].

Chapter 2

Prerequisites

In this chapter, we provide some concepts and results we will need for the rest of this work.

2.1 Basic Graph Theory Terminology

For the prerequisites from graph theory we refer to [10].

Definition 2.1.1. A *graph* G is a triple (V, E, τ) where V is a vertex set, E is an edge set and τ is the incidence function that associates to each edge an unordered pair of vertices. If $\tau(e) = \{a, b\}$, then edge e is said to be incident to vertices a and b, and we say that vertices a and b are adjacent. We will indicate adjacency of vertices a and b by $a \sim b$.
If a and b are not distinct, then we say e is a *loop*. Edges incident to the same pair of vertices are called *multiple edges*. A graph that has neither multiple edges nor loops is a *simple graph*. For simple graphs, there is no ambiguity in referring to an edge e with endpoints a and b as $e = \{a, b\}$ or just $e = ab$. In other words, the incidence function may be omitted for simple graphs. A graph is *finite* if V and E are both finite otherwise it is *infinite*. Unless stated otherwise, we deal with *finite* graphs. The *degree* of a vertex v is the number of edges that are incident to it, with loops counting twice. We shall denote the degree of a vertex v as $\deg(v)$. If every vertex of a graph has the same degree d, we say the graph is *d-regular*.

Unless otherwise stated, in this document we shall be dealing with simple graphs.

Definition 2.1.2. A *walk* in a graph is a sequence $W = x_0e_1x_1e_2x_2e_3 \dots e_nx_n$ where $x_0, x_1, x_2, \dots, x_n \in V$, and $e_1, e_2, e_3, \dots, e_n \in E$ and the endpoints of edge e_i are x_{i-1} and x_i for all $i = 1, \dots, n$. Note that vertices and edges in the sequence need not all be distinct. The walk W is *closed* if the initial vertex and the final vertex are the same. A *path* is a walk that has no repeated vertices. A closed walk with no repeated vertices, except the initial and final vertex is called a *cycle*. The *length* of a walk is the number of edges appearing in the sequence. The *distance* between two vertices is the length of a shortest path between them. The *diameter* of a graph is the largest distance between any pair of vertices in the graph. The *girth* of a graph is the length of a shortest cycle contained in the graph. A graph is *connected* if there exists a path between any pair of vertices in the graph.

2.2 Graph Matrices

For the prerequisites from algebraic graph theory, we refer to [9, 35].

Often it is useful to represent a graph as a matrix. We can make several deductions from the graph by studying its matrix representation. We shall look at two ways of representing a graph by a matrix, namely, *adjacency* matrix representation and *Laplacian* matrix representation. In both cases, we assume a fixed ordering of the vertices say $1, 2, 3, ..., n$.

Definition 2.2.1. The *adjacency matrix* of a graph G, denoted by $A(G)$ or just A if the graph is unambiguous, is the matrix $A = [A_{ij}]$ whose rows and columns are indexed by the vertices of G, with A_{ij} being the number of edges whose endpoints are $\{i, j\}$. So for simple graphs, $A_{i,j} = 1$ if $i \sim j$ and 0 otherwise. It is worth noting that A is real and symmetric.

Definition 2.2.2. The *Laplacian matrix* of a graph G, usually denoted as $L(G)$ or simply L, is the matrix $L = D - A$, where D is the diagonal matrix of vertex degrees, and A is the adjacency matrix of G. Thus, L is an $n \times n$ matrix with entries $\ell_{i,j}$ given by

$$\ell_{i,j} := \begin{cases} \deg(i) & \text{if } i = j, \\ -1 & \text{if } \{i, j\} \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Remark 2.2.3. We remark here that if G is δ-regular, then $D = \delta I$, so $L = \delta I - A$. Hence the eigenvectors of L are the same as those of A, and the eigenvalue θ of A corresponds to the eigenvalue $\delta - \theta$ for L. Thus results for a regular graph G that depend on its adjacency matrix A can be phrased in terms of its Laplacian matrix L.

Most of our results pertain to eigenvalues of these graph matrices. Recall that a number λ is an eigenvalue of a square matrix M and a non-zero vector $\mathbf{x}$ is an eigenvector if $M\mathbf{x} = \lambda\mathbf{x}$. We say $\mathbf{x}$ is a λ-*eigenvector* for M. The union of the zero vector and the set of λ-eigenvectors is referred to as the λ eigenspace. The set of eigenvalues of a matrix M is called the spectrum, $\text{ev}(M)$, of M. The eigenvalues of a graph are the eigenvalues of an associated matrix of the graph. We shall refer to the eigenvalues of the adjacency matrix of G as the *adjacency eigenvalues* of G, while *Laplacian eigenvalues* represent the eigenvalues of the Laplacian matrix of G. Traditionally, to find the eigenvectors of a matrix M, we first factor the determinant of $M - \lambda I$ to find the eigenvalues. Another way to find eigenvectors and eigenvalues of a matrix of a graph G is to translate the definition of eigenvalues into a condition at each vertex of G. This approach has the advantage that one can deduce the eigenvectors from the structure of the graph. We shall formulate it in a form of a proposition. Think of the entry x_i of $\mathbf{x}$ as a weight on vertex $i \in V$.

Proposition 2.2.4. *Let A and L be respectively, the adjacency and Laplacian matrix of a simple graph G with vertex set $V(G) = \{1, 2, \ldots, n\}$, and $\mathbf{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$ and $\lambda, \mu \in \mathbb{R}$. Then*

- *$A\mathbf{x} = \lambda\mathbf{x}$ if and only if $\sum_{j\sim i} x_j = \lambda x_i$ for all i.*
- *$L\mathbf{x} = \mu\mathbf{x}$ if and only if $\sum_{j\sim i} x_j = (deg(i) - \mu)x_i$ for all i.*

We recall the following results about real symmetric matrices.

Theorem 2.2.5. *[35] Let M be a real symmetric matrix.*

i. If $\mathbf{u}$ and $\mathbf{v}$ are eigenvectors of M corresponding to different eigenvalues, then $\mathbf{u}$ and $\mathbf{v}$ are orthogonal.

ii. The eigenvalues of M are real numbers.

iii. (Spectral decomposition) Suppose $\mathbf{v}_i$ is a λ_i-eigenvector for M. Then M can be written as

$$M = \sum_{\lambda_i \in \mathrm{ev}(M)} \lambda_i E_{\lambda_i},$$

where $E_{\lambda_i} = \mathbf{v}_i \mathbf{v}_i^T$ is a projection matrix onto the λ_i eigenspace.

Proof:

i. Suppose $M\mathbf{u} = \lambda\mathbf{u}$ and $M\mathbf{v} = \tau\mathbf{v}$. Since M is symmetric, we have

$$\mathbf{v}^T M\mathbf{u} = (\mathbf{u}^T M\mathbf{v})^T.$$

This implies

$$\lambda\mathbf{v}^T\mathbf{u} = (\tau\mathbf{u}^T\mathbf{v})^T = \tau\mathbf{v}^T\mathbf{u}.$$

Simplifying these equations, we get

$$(\lambda - \tau)\mathbf{v}^T\mathbf{u} = 0.$$

Since $\lambda - \tau \neq 0$, it follows that $\mathbf{v}^T\mathbf{u} = 0$, proving the claim.

ii. Suppose $M\mathbf{u} = \lambda\mathbf{u}$, and take its complex conjugate to get $M\bar{\mathbf{u}} = \bar{\lambda}\bar{\mathbf{u}}$. So both $\mathbf{u}$ and $\bar{\mathbf{u}}$ are eigenvectors of M. But then, since an eigenvector is non zero, we have $\mathbf{u}^T\bar{\mathbf{u}} > 0$. And so by part (i.), $\mathbf{u}$ and $\bar{\mathbf{u}}$ cannot have different eigenvalues, that is $\lambda = \bar{\lambda}$, proving the claim.

iii. M is symmetric if and only if M is orthogonally diagonalizable, that is, $M = QDQ^{-1}$, where $Q^{-1} = Q^T$. Then

$$\begin{aligned} M &= QDQ^T \\ &= [\mathbf{v}_1 \dots \mathbf{v}_n] \begin{bmatrix} \lambda_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \lambda_n \end{bmatrix} \begin{bmatrix} \mathbf{v}_1^T \\ \vdots \\ \mathbf{v}_n^T \end{bmatrix} \\ &= [\mathbf{v}_1\lambda_1 \dots \mathbf{v}_n\lambda_n] \begin{bmatrix} \mathbf{v}_1^T \\ \vdots \\ \mathbf{v}_n^T \end{bmatrix} \\ &= \lambda_1\mathbf{v}_1\mathbf{v}_1^T + \dots + \lambda_n\mathbf{v}_n\mathbf{v}_n^T \\ &= \sum_{\lambda_i \in \text{ev}(M)} \lambda_i\mathbf{v}_i\mathbf{v}_i^T. \end{aligned}$$

Moreover, observe that for $\mathbf{x} \in \mathbb{R}^n$, we have $\mathbf{v}_i\mathbf{v}_i^T\mathbf{x} = \mathbf{v}_i(\mathbf{v}_i \cdot \mathbf{x}) = \text{proj}_{\mathbf{v}_i}\mathbf{x}$.

∎

Theorem 2.2.5 iii can be generalized. For p a polynomial, we have that $p(M) = \sum_{\lambda_i \in \text{ev}(M)} p(\lambda_i)E_{\lambda_i}$. We shall revisit this in Lemma 2.2.16.

Definition 2.2.6. The *trace* $\text{tr}(A)$ of a matrix A is the sum of its diagonal entries.

One way to look at the entry A_{ij} of the adjacency matrix A of a graph is as the number of walks of length one (that is, the number of edges) from vertex i to vertex j. This way of looking at the adjacency matrix generalizes to walks of higher length.

Proposition 2.2.7. *If A is the adjacency matrix of a graph G, then $(A^k)_{ij}$ is the number of walks of length k from vertex i to vertex j.*

The following is then immediate.

Corollary 2.2.8. *The number of closed walks of length k in a graph with adjacency matrix A is $\text{tr}(A^k)$.*

Proposition 2.2.9. *Let A be an $n \times n$ matrix with eigenvalues $\theta_1, \theta_2, \dots, \theta_n$. Then $\text{tr}(A) = \sum_{i=1}^n \theta_i$.*

Now since the trace of the adjacency matrix A of a simple graph is zero, we can deduce that the eigenvalues of an adjacency matrix sum to zero, and that unless $A = 0$, there are both positive and negative eigenvalues of A.

Proposition 2.2.10. *Let A be an $n \times n$ matrix, and a non-zero vector $\mathbf{x} \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}$. If*

$$A\mathbf{x} = \lambda\mathbf{x} \quad \textit{then} \quad A^k\mathbf{x} = \lambda^k\mathbf{x}.$$

That is, the eigenvalues of all powers of A are determined by the eigenvalues of A. Combining Propositions 2.2.9 and 2.2.10 we obtain the following useful result.

Corollary 2.2.11. *Let A be an $n \times n$ matrix with eigenvalues $\theta_1, \theta_2, \dots, \theta_n$. Then $\mathrm{tr}(A^k) = \sum_{i=1}^{n} \theta_i^k$.*

Using Corollaries 2.2.8 and 2.2.11, we see that we can deduce the number of closed walks of any length in a graph G from the spectrum of A. This observation is captured in the following.

Proposition 2.2.12. *Let A be the adjacency matrix of a graph of order n with eigenvalues $\theta_1, \theta_2, \dots, \theta_n$. Then the number of closed walks of length k is $\mathrm{tr}(A^k) = \sum_{i=1}^{n} \theta_i^k$.*

Theorem 2.2.13. *(Perron-Frobenius [35]) Let A be the adjacency matrix of a connected graph G with eigenvalues $\theta_1, \theta_2, \dots, \theta_n$ such that $\theta_1 \geq \theta_2 \geq \cdots \geq \theta_n$ and corresponding eigenvectors $\mathbf{x_1}, \mathbf{x_2}, \dots, \mathbf{x_n}$. Then*

- *θ_1 is positive and simple (that is, θ_1 has algebraic multiplicity 1) with eigenvector $\mathbf{x_1}$ with all positive entries (up to a multiplication by a positive scalar)*
- *$\theta_1 \geq |\theta_i|$ for all $i = 2, \dots, n$.*

The value of θ_1 in Theorem 2.2.13 is often called the *spectral radius* or the *Perron eigenvalue* of matrix A. One thing we can easily deduce from the above is that if $\theta_1, \theta_2, \dots \theta_n$ are the eigenvalues of A and $\theta_1 \geq \theta_2 \geq \cdots \geq \theta_n$, then $|\theta_n| \leq \theta_1$. The equality holds if and only if the graph is bipartite [34].

Given that M is a positive $n \times n$ matrix, we note that $M\mathbf{1}$ is a vector whose ith entry comprises of the sum of entries in row i of M. Thus if M has the property that the entries in every row sum to the same number δ, then $M\mathbf{1} = \delta\mathbf{1}$. That is, δ is an eigenvalue of M with $\mathbf{1}$ as its corresponding eigenvector. Since $\mathbf{1}$ is a positive vector, using Theorem 2.2.13, the following result is proven.

Proposition 2.2.14. *Let M be a positive $n \times n$ matrix with the property that the entries in every row sum to the same number, δ. Then δ is the Perron eigenvalue of M.*

Since in this work, most graphs are regular, the following is worth stating.

Proposition 2.2.15. *A connected graph is δ-regular if and only if $\mathbf{1}$ is an eigenvector for its adjacency matrix. In this case, the largest eigenvalue is δ and it is simple.*

We can evaluate a polynomial at a square matrix M. Let $p(x) \in \mathbb{R}[x]$ be a polynomial of degree k. Then $p(M)$ is the matrix $p(M) = a_k M^k + a_{k-1}M^{k-1} + \cdots + a_1 M + a_0 I$. The following is worth noting.

Lemma 2.2.16. *Let $p(x) \in \mathbb{R}[x]$ be a polynomial of degree k and let M be an $n \times n$ matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$ (including multiplicities).*

i. Then the matrix $p(M)$ has eigenvalues $p(\lambda_1), \ldots, p(\lambda_n)$.

ii. If M has the property that the entries in every row sum to the same number, d, then $p(M)$ has the property that the entries in every row sum to the same number, $p(d)$.

Proof:

i. Suppose $M\mathbf{x} = \lambda\mathbf{x}$. Then $M^2\mathbf{x} = M(\lambda\mathbf{x}) = \lambda(M\mathbf{x}) = \lambda^2\mathbf{x}$. Inductively, we have that for $k \in \mathbb{N}$,

$$M^k\mathbf{x} = \lambda^k\mathbf{x}. \tag{2.2.1}$$

Now bearing (2.2.1) in mind, we have

$$\begin{aligned} p(M)\mathbf{x} &= (a_k M^k + a_{k-1}M^{k-1} + \cdots + a_1 M + a_0 I)\mathbf{x} \\ &= a_k M^k\mathbf{x} + a_{k-1}M^{k-1}\mathbf{x} + \cdots + a_1 M\mathbf{x} + a_0 I\mathbf{x} \\ &= a_k\lambda^k\mathbf{x} + a_{k-1}\lambda^{k-1}\mathbf{x} + \cdots + a_1\lambda\mathbf{x} + a_0\mathbf{x} \\ &= p(\lambda)\mathbf{x}. \end{aligned}$$

ii. Recall that if $M = [a_{ij}]$, then $M^2 = [c_{ij}]$ where

$$c_{ij} = a_{i1}a_{1j} + a_{i2}a_{2j} + \cdots + a_{in}a_{nj} = \sum_{k=1}^{n} a_{ik}a_{kj}.$$

Note that the sum of entries of row i of M is $\sum_{j=1}^{n} a_{ij} = d$, for all $i = 1, \ldots, n$ by the hypothesis. Now sum of entries of row i of M^2 is

$$\begin{aligned} \sum_{j=1}^{n} c_{ij} &= \sum_{j=1}^{n}\sum_{k=1}^{n} a_{ik}a_{kj} \\ &= \sum_{k=1}^{n} a_{ik}\sum_{j=1}^{n} a_{kj} \end{aligned}$$

$$= \sum_{k=1}^{n} a_{ik} d = d^2.$$

Inductively, the sum of entries of row i of M^k is d^k, for all rows $i = 1, \ldots, n$. It is therefore clear that the sum of entries of row i of τM^k is τd^k, for any $\tau \in \mathbb{R}$. Hence the sum of entries of row i of $p(M)$ is $p(d)$, for all $i = 1, \ldots, n$.

∎

2.3 Rayleigh Quotients

Rayleigh quotients is a tool from linear algebra that proves very useful in our understanding of *interlacing* (to be defined later) and its applications. Consider a real symmetric $n \times n$ matrix M with eigenvalues $\lambda_1, \ldots, \lambda_n$ with $\lambda_1 \geq \cdots \geq \lambda_n$ whose respective eigenvectors are $\mathbf{u_1}, \ldots, \mathbf{u_n}$. Recall that these eigenvalues are real and that we may assume $\mathbf{u_1}, \ldots, \mathbf{u_n}$ is an orthonormal set. Hence, for any $\mathbf{x} \in \mathbb{R}^n$, there exists $a_1, a_2, \ldots, a_n \in \mathbb{R}$ such that $\mathbf{x} = a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n}$. Then

$$\begin{aligned}
\frac{\mathbf{x}^T M \mathbf{x}}{\mathbf{x}^T \mathbf{x}} &= \frac{(a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n})^T M (a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n})}{(a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n})^T (a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n})} \\
&= \frac{(a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n})^T (a_1 M\mathbf{u_1} + a_2 M\mathbf{u_2} + \cdots + a_n M\mathbf{u_n})}{(a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n})^T (a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n})} \\
&= \frac{(a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n})^T (a_1\lambda_1\mathbf{u_1} + a_2\lambda_2\mathbf{u_2} + \cdots + a_n\lambda_n\mathbf{u_n})}{(a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n})^T (a_1\mathbf{u_1} + a_2\mathbf{u_2} + \cdots + a_n\mathbf{u_n})} \\
&= \frac{(\lambda_1 a_1^2 + \lambda_2 a_2^2 + \cdots + \lambda_n a_n^2)}{a_1^2 + a_2^2 + \cdots + a_n^2} = \frac{(\lambda_1 a_1^2 + \lambda_2 a_2^2 + \cdots + \lambda_n a_n^2)}{||\mathbf{x}||^2}
\end{aligned}$$

Thus if we fix $||\mathbf{x}||^2$, then we can determine the maximum and the minimum of the above quotient on the corresponding region in $\mathbb{R}^n$. A maximum is obtained by setting $a_i = 0$ for $2 \leq i \leq n$. In other words, $\mathbf{x} = a_1\mathbf{u_1}$. Similarly, a minimum is obtained when $\mathbf{x} = a_n\mathbf{u}_n$. The following result is the general bound based on the above idea.

Lemma 2.3.1. *(Rayleigh Inequalities) Let M be a real symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$, with respective orthonormal eigenvectors $\mathbf{u_1}, \ldots, \mathbf{u_n}$. Let Y be the set of nonzero vectors orthogonal to $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_{j-1}\}$, and Z be the set of nonzero vectors orthogonal to $\{\mathbf{u}_{j+1}, \mathbf{u}_{j+2}, \ldots, \mathbf{u}_n\}$.*

i. Then

$$\frac{\mathbf{y}^T M \mathbf{y}}{\mathbf{y}^T \mathbf{y}} \leq \lambda_j \leq \frac{\mathbf{z}^T M \mathbf{z}}{\mathbf{z}^T \mathbf{z}}$$

for any $\mathbf{y} \in Y$ and $\mathbf{z} \in Z$.

ii. If $\mathbf{y}$ *is a* λ_j*-eigenvector for* M*, then* $\frac{\mathbf{y}^T M\mathbf{y}}{\mathbf{y}^T\mathbf{y}} = \lambda_j$*. If* $\mathbf{z}$ *is a* λ_j*-eigenvector for* M*, then* $\lambda_j = \frac{\mathbf{z}^T M\mathbf{z}}{\mathbf{z}^T\mathbf{z}}$.

Thus any $\mathbf{y} \in Y$ gives a lower bound on λ_j, and any $\mathbf{z} \in Z$ gives an upper bound on λ_j. A commonly seen special form of Lemma 2.3.1 is below.

Corollary 2.3.2. *Let* M *be a real symmetric* $n \times n$ *matrix with eigenvalues* $\lambda_1 \geq \cdots \geq \lambda_n$*. Then*

$$\lambda_n \leq \frac{\mathbf{x}^T M\mathbf{x}}{\mathbf{x}^T\mathbf{x}} \qquad \text{and} \qquad \frac{\mathbf{x}^T M\mathbf{x}}{\mathbf{x}^T\mathbf{x}} \leq \lambda_1, \tag{2.3.1}$$

for any $\mathbf{x} \neq 0$.

For a Laplacian matrix, we have the following.

Lemma 2.3.3 (Quadratic Form for the Laplacian matrix)**.** *Let* L *be the Laplacian matrix of a graph* G *of order* n*. For any vector* $\mathbf{x} \in \mathbb{R}^n$*,*

$$\mathbf{x}^T L\mathbf{x} = \sum_{\{i,j\}\in E} (x_i - x_j)^2. \tag{2.3.2}$$

Proof: We have

$$\mathbf{x}^T L\mathbf{x} = \sum_{i,j=1} \ell_{i,j} x_i x_j = \sum_{i=1}^{n} deg(i) x_i^2 - 2 \sum_{\{i,j\}\in E} x_i x_j,$$

which simplifies to

$$\sum_{\{i,j\}\in E} (x_i - x_j)^2.$$

∎

The Laplacian eigenvalues are all non-negative and the constant vector $\mathbf{1}$ is an eigenvector for the zero eigenvalue.

In particular, we will utilize the following form of Corollary 2.3.2.

Corollary 2.3.4. *Let* G *be a connected graph of order* n *with Laplacian matrix* L *and Laplacian eigenvalues* $0 = \mu_1 \leq \mu_2 \leq \cdots \leq \mu_n$*. Then*

$$\mu_2 \leq \frac{\mathbf{x}^T L\mathbf{x}}{\mathbf{x}^T\mathbf{x}} \qquad \text{and} \qquad \frac{\mathbf{x}^T L\mathbf{x}}{\mathbf{x}^T\mathbf{x}} \leq \mu_n, \tag{2.3.3}$$

for any $\mathbf{x}$ *orthogonal to the constant vector* $\mathbf{1}$.

2.4 Interlacing

Interlacing is an important tool we will be using throughout this thesis. The principal form of interlacing was attributed to Cauchy [42] while the general form is due to Courant and Hilbert [22]. The application of this tool to graphs was popularized by Haemers [42]. Interlacing relates the spectrum of a graph to induced subgraphs or other structures in the graph.

Definition 2.4.1. Consider sequences $(\mu_1, \mu_2, \ldots, \mu_k)$ and $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ with $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_k$ and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ where $k < n$. We say the first sequence *interlaces* the second sequence if $\lambda_i \geq \mu_i \geq \lambda_{n-k+i}$ for $i = 1, \ldots, k$. Moreover, the interlacing is said to be *tight* if for some ℓ, $1 \leq \ell \leq l$, we have $\lambda_i = \mu_i$ for $i = 1, \ldots, l$ and $\mu_i = \lambda_{n-k+i}$ for $i = l+1, \ldots, k$.

For instance, if $k = n-1$, then sequence $(\mu_1, \mu_2, \ldots, \mu_{n-1})$ interlaces the sequence $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ if and only if

$$\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \lambda_n.$$

Let M be a real symmetric $n \times n$ matrix. A *principal submatrix* N of M is a matrix obtained from M by deleting row i and column i of M for some values of i. In other words, for some $S \subseteq \{1, 2, \ldots, n\}$, matrix N is the submatrix of M that contains only rows and columns indexed by S. Another useful way of considering the principal submatrix N is as follows. Let R be the matrix obtained from the $n \times n$ identity matrix I by keeping only the columns of I that correspond to S. Then $N = R^T MR$. The following result is a special case of an interlacing theorem. It is usually called *Principal Interlacing*.

Theorem 2.4.2. *(Principal Interlacing [42]) Let M be a real symmetric $n \times n$ matrix, and let R be an $n \times k$ submatrix of the $n \times n$ identity matrix. Then the eigenvalues of $R^T MR$ interlace the eigenvalues of M.*

The principal interlacing follows as a corollary of the interlacing theorem to be proved later.

Remark 2.4.3. Theorem 2.4.2 is also true for Hermitian matrices.

The principal interlacing theorem simply says that the eigenvalues of a principal submatrix interlace the eigenvalues of the matrix. Let G be a graph and H an induced subgraph of G. Let $V(G) = \{1, 2, \ldots, n\}$ and $V(H) = S$, for some $S \subseteq V(G)$. Let M be the adjacency matrix of G, and R the submatrix of $I_{n\times n}$ consisting of the columns of $I_{n\times n}$ indexed by S. Then $R^T MR$ is the adjacency matrix of H (and a principal submatrix of M). Theorem 2.4.2 tells us that the eigenvalues of H (that is, eigenvalues of $R^T MR$) interlace the eigenvalues of G (that is, eigenvalues of M).

We provide a very simple application of interlacing. Let G be a simple graph of order n with at least one edge. It is clear that K_2 is an induced subgraph of G. The adjacency eigenvalues of K_2 are 1 and -1. Suppose G has adjacency eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, then by Theorem 2.4.2, the sequence $(1, -1)$ interlaces the sequence $(\lambda_1, \lambda_2, \ldots, \lambda_n)$. That is, $\lambda_1 \geq 1 \geq \lambda_{n-1}$ and $\lambda_2 \geq -1 \geq \lambda_n$. In particular, we have $\lambda_1 \geq 1$ and $-1 \geq \lambda_n$. Thus we have established the following.

Lemma 2.4.4. *Let G be a simple graph of order n with at least one edge. Suppose G has adjacency eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then $\lambda_n \leq -1$ and $\lambda_1 \geq 1$.*

We now give a generalization of the Principal Interlacing Theorem, Theorem 2.4.2. We note that in Theorem 2.4.2, matrix R satisfies $R^T R = I$, and it turns out that this property is sufficient. The next result tells us more about the interlacing of the eigenvalues of M by the eigenvalues of a matrix $N = R^T M R$.

Theorem 2.4.5. *(Interlacing Theorem [35, 42]) Let M be a real symmetric $n \times n$ matrix, R a real $n \times k$ matrix such that $R^T R = I$, and $N = R^T M R$ for $n \geq k$. Let the eigenvalues of M be $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ with corresponding orthonormal eigenvectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$, and let the eigenvalues of N be $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_k$ with corresponding orthonormal eigenvectors $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_k$. Then the following hold.*

i. The eigenvalues of N interlace the eigenvalues of M.

ii. If $\mu_i = \lambda_i$ (or $\mu_i = \lambda_{n-k+i}$), then there exists $\mathbf{u} \in \mathbb{R}^k$ with $N\mathbf{u} = \mu_i \mathbf{u}$ and $M(R\mathbf{u}) = \mu_i(R\mathbf{u})$.

iii. If for some ℓ we have $\mu_i = \lambda_i$ for $i = 1, \ldots, \ell$ (or $\mu_i = \lambda_{n-k+i}$ for $i = \ell, \ldots, k$), then $M(R\mathbf{u}_i) = \mu_i(R\mathbf{u}_i)$ for $i = 1, \ldots, \ell$ ($i = \ell, \ldots, k$ respectively).

iv. If the interlacing is tight, then $MR = RN$.

Proof:

i. Let $\langle \mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_i \rangle$ denote the span of $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_i$. Fix $i \in \{1, \ldots, k\}$. We first show $\mu_i \leq \lambda_i$. We have that $\langle \mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_i \rangle \cap \langle R^T \mathbf{v}_1, R^T \mathbf{v}_2, \ldots, R^T \mathbf{v}_{i-1} \rangle^\perp$ is the intersection of a subspace of dimension i and a subspace of dimension $n - i + 1$, so it contains a nonzero vector. Let $\mathbf{z_i}$ be such a vector. Certainly $\mathbf{z_i} \in \langle \mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_i \rangle$. For all $j < i$, we have that $\mathbf{z_i} \perp R^T \mathbf{v}_j$, so $\mathbf{z_i}^T R^T \mathbf{v}_j = 0$ and $(R\mathbf{z_i})^T \mathbf{v}_j = 0$. Therefore, $R\mathbf{z_i} \in \langle \mathbf{v}_i, \ldots, \mathbf{v}_n \rangle$. Then using Lemma 2.3.1, $\mathbf{z_i} \in \langle \mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_i \rangle = \langle \mathbf{u}_{i+1}, \mathbf{u}_{i+2}, \ldots, \mathbf{u}_k \rangle^\perp$ implies

$$\mu_i \leq \frac{\mathbf{z_i}^T N \mathbf{z_i}}{\mathbf{z_i}^T \mathbf{z_i}}.$$

Also $R\mathbf{z_i} \in \langle \mathbf{v}_i, \ldots, \mathbf{v}_n \rangle = \langle \mathbf{v}_1, \ldots, \mathbf{v}_{i-1} \rangle^{\perp}$ implies

$$\frac{(R\mathbf{z_i})^T M (R\mathbf{z_i})}{(R\mathbf{z_i})^T (R\mathbf{z_i})} \leq \lambda_i.$$

And hence we have

$$\mu_i \leq \frac{\mathbf{z_i}^T N \mathbf{z_i}}{\mathbf{z_i}^T \mathbf{z_i}} = \frac{\mathbf{z_i}^T R^T M R \mathbf{z_i}}{\mathbf{z_i}^T R^T R \mathbf{z_i}} = \frac{(R\mathbf{z_i})^T M (R\mathbf{z_i})}{(R\mathbf{z_i})^T (R\mathbf{z_i})} \leq \lambda_i, \tag{2.4.1}$$

that is, $\mu_i \leq \lambda_i$.

We prove the other assertion, that is, $\mu_i \geq \lambda_{n-k+i}$, using the same argument with $-M$ and $-N$ (or applying (2.4.1) to $-M$ and $-N$). Note that the eigenvalues of $-M$ are $-\lambda_n \geq \cdots \geq -\lambda_2 \geq -\lambda_1$, renamed as $\lambda'_1 \geq \lambda'_2 \geq \cdots \geq \lambda'_n$, so that $\lambda'_i = -\lambda_{n-i+1}$. Similarly, the eigenvalues of $-N$ are $-\mu_k \geq \cdots \geq -\mu_1$, renamed as $\mu'_1 \geq \mu'_2 \geq \cdots \geq \mu'_k$ so that $\mu'_i = -\mu_{k-i+1}$. Now applying (2.4.1) to $-M$ and $-N$, we have that

$$\begin{aligned} \mu'_i &\leq \lambda'_i \text{ for all } i = 1, \ldots, k \\ -\mu_{k-i+1} &\leq -\lambda_{n-i+1} \text{ for all } i = 1, \ldots, k \\ -\mu_j &\leq -\lambda_{n-k+j} \text{ for all } j = k, \ldots, 1 \\ \mu_j &\geq \lambda_{n-k+j} \text{ for all } j = 1, \ldots, k. \end{aligned}$$

Hence $\mu_i \geq \lambda_{n-k+i}$.

ii. If $\mu_i = \lambda_i$, that is,

$$\mu_i = \frac{z_i^T N z_i}{z_i^T z_i} = \frac{z_i^T R^T M R z_i}{z_i^T R^T R z_i} = \frac{(Rz_i)^T M (Rz_i)}{(Rz_i)^T (Rz_i)} = \lambda_i,$$

then using the equality condition of Lemma 2.3.1, z_i is a μ_i-eigenvector of N and Rz_i is a λ_i-eigenvector of M. We note that this does not necessarily mean that $z_i = \mathbf{u}_i$.

iii. We prove (iii) by induction on ℓ. If $\ell = 1$, then we can take z_1 in (2.4.1) to be $z_1 = \mathbf{u}_1$ and deduce that $MR\mathbf{u}_1 = \lambda_1 R\mathbf{u}_1$. If we assume that $MR\mathbf{u}_i = \lambda_i R\mathbf{u}_i$ for $i = 1, \ldots, \ell - 1$, then we may assume $\mathbf{v}_i = R\mathbf{u}_i$ for $i = 1, \ldots, \ell - 1$. Hence we can choose $z_\ell = \mathbf{u}_\ell$, but in proving (ii) we saw that Rz_ℓ is a λ_ℓ-eigenvector of M. The other assertion follows from applying the same argument with $-M$ and $-N$.

iv. If $\mu_i = \lambda_i$ for $i = 1, \ldots, \ell$ and $\mu_i = \lambda_{n-k+i}$ for $i = \ell+1, \ldots, k$, then by part (iii), we have that $\mu_1, \ldots, \mu_k$ are eigenvalues for M with corresponding eigenvectors

$R\mathbf{u}_1, \ldots, R\mathbf{u}_k$. That is, for all i, $MR\mathbf{u}_i = \mu_i R\mathbf{u}_i$. Using also the fact that $N\mathbf{u}_i = \mu_i \mathbf{u}_i$, we have that for all i,

$$RN\mathbf{u}_i = R\mu_i\mathbf{u}_i = \mu_i R\mathbf{u}_i = MR\mathbf{u}_i,$$

and since $\mathbf{u}_1, \ldots, \mathbf{u}_k$ is a basis for $\mathbb{R}^k$, this implies that $RN = MR$.

∎

Remark 2.4.6. If we take $R = [I \quad O]^T$, then $N = R^T MR$ is a principal submatrix of M and so Theorem 2.4.2 follows as a corollary to Theorem 2.4.5.

2.5 Quotient Matrices

In this section, we define the quotient matrix of a graph with respect to a particular partition of its vertex set. Our goal is to show by Theorem 2.4.5 that the eigenvalues of this quotient matrix interlace the eigenvalues of the adjacency matrix of the graph.

Let $\pi = \{V_1, \ldots, V_k\}$ be a partition of the vertex set V of a graph G. We may choose an ordering of V such that this partition induces a block partition of the adjacency matrix A of the graph. Let $A_{(ij)}$ be the submatrix of A whose rows correspond to V_i and whose columns correspond to V_j

$$A = \left[\begin{array}{c|c|c} A_{(1,1)} & \cdots & A_{(1,k)} \\ \hline \vdots & & \vdots \\ \hline A_{(k,1)} & \cdots & A_{(k,k)} \end{array}\right] \tag{2.5.1}$$

Recall that the *characteristic matrix* P of the partition π is an $n \times k$ matrix whose jth-column is the characteristic vector of the set V_j.

Definition 2.5.1. Let G be a graph and $\pi = \{V_1, \ldots, V_k\}$ a partition of $V(G)$ with characteristic matrix P. The *quotient matrix* of G with respect to the partition π is a matrix, denoted by $B = A(G/\pi)$, whose entry B_{ij} is the average row-sum of the block $A_{(ij)}$, that is, the sum of all entries in block $A_{(ij)}$ divided by the number of rows. Thus

$$B_{i,j} = \frac{1}{|V_i|}\mathbf{1}^T A_{(i,j)}\mathbf{1} = \frac{1}{|V_i|}(P^T AP)_{i,j}.$$

Note that $B = A(G/\pi)$ is not necessarily symmetric, and it can have nonzero entries on the diagonal. Hence, B is the adjacency matrix of a directed graph with $\{V_1, \ldots, V_k\}$ as vertex set, and B_{ij} arcs from V_i to V_j.

Indeed the quotient matrix of a graph can be considered as an application of the following definition of quotient matrix of a symmetric matrix. Suppose A is a real symmetric matrix whose rows and columns are indexed by $V = \{1, \dots, n\}$. Let $\pi = \{V_1, \dots, V_k\}$ be a partition of V. Let A be partitioned according to π as in (2.5.1). The *quotient matrix* of A with respect to the partition π is the matrix $B = (b_{ij})$, where b_{ij} is the average row sum of block $A_{(ij)}$ of matrix A.

Definition 2.5.2. A partition $\pi = \{V_1, \dots, V_k\}$ of the vertex set of a graph G is *equitable or regular* if there are constants b_{ij} such that every vertex in V_i is adjacent to exactly b_{ij} vertices of V_j. In other words, each vertex $v \in V_i$, has the same number, namely, b_{ij}, of neighbours in V_j.

We have the following characterisation of equitable partitions.

Proposition 2.5.3. *[35] Let P be the characteristic matrix of a partition $\pi = \{V_1, \dots, V_k\}$ of the vertex set of a graph G. Partition π is equitable if and only if there exists a matrix B with $AP = PB$. If this is the case then $B = A(G/\pi)$.*

We can get a formula for B in Definition 2.5.1. We note that $(P^TAP)_{i,j}$ is the number of edges between vertices of V_i and V_j, and $|V_i| = (P^TP)_{i,i}$. Hence from Definition (2.5.1), $B_{i,j} = (P^TP)^{-1}_{i,i}(P^TAP)_{i,j}$, which is the average number of edges from a vertex in part V_i to vertices in part V_j of the partition π. We also know that P^TP is a diagonal matrix. This proves the following result.

Proposition 2.5.4. *[35] Let $B = A(G/\pi)$ be the quotient matrix of a graph G with respect to a partition π of $V(G)$, and let P be the characteristic matrix of the partition. Then $B = (P^TP)^{-1}P^TAP$.*

Now let us get to our main interest. The following result, which is actually a consequence of Theorem 2.4.5, underlines several other results we will be showing.

Theorem 2.5.5. *[35, 42] Let G be a graph and $\pi = \{V_1, \dots, V_k\}$ a partition of $V(G)$. The eigenvalues of the quotient matrix $B = A(G/\pi)$ interlace the eigenvalues of the adjacency matrix A of G. If the interlacing is tight, then the partition π is equitable.*

Proof: Let P be the characteristic matrix of the partition π. The matrix P^TP is a diagonal matrix with positive diagonal entries, so we can set $R = P(P^TP)^{-1/2}$. We have

$$R^TR = (P(P^TP)^{-1/2})^TP(P^TP)^{-1/2} = (P^TP)^{-1/2}P^TP(P^TP)^{-1/2} = I.$$

Let $N = R^TAR$. We have

$$N = R^TAR = (P^TP)^{-1/2}P^TAP(P^TP)^{-1/2} = (P^TP)^{1/2}((P^TP)^{-1}P^TAP)(P^TP)^{-1/2}.$$

Thus, matrix N is similar to matrix $(P^TP)^{-1}P^TAP = B$ and has the same eigenvalues. Now using Theorem 2.4.5, we have that the eigenvalues of N interlace the eigenvalues of A, and if the interlacing is tight, then $AR = RN$. Thus the eigenvalues of the quotient matrix B interlace the eigenvalues of A. Moreover, for tight interlacing, we have

$$
\begin{aligned}
AR = RN &\Leftrightarrow AP(P^TP)^{-1/2} = P(P^TP)^{-1/2}R^TAR \\
&\Leftrightarrow AP(P^TP)^{-1/2} = P(P^TP)^{-1/2}(P(P^TP)^{-1/2})^TAP(P^TP)^{-1/2} \\
&\Leftrightarrow AP(P^TP)^{-1/2}(P^TP)^{1/2} = P(P^TP)^{-1/2}(P(P^TP)^{-1/2})^TAP(P^TP)^{-1/2}(P^TP)^{1/2} \\
&\Leftrightarrow AP = P(P^TP)^{-1/2}(P^TP)^{-1/2}P^TAP \\
&\Leftrightarrow AP = P(P^TP)^{-1}P^TAP \\
&\Leftrightarrow AP = PB,
\end{aligned}
$$

which shows the partition is equitable by Proposition 2.5.3. ∎

Chapter 3

Previous Work on the k-Independence Number

In this chapter we discuss previous results on the subject matter. We pay close attention to the algebraic techniques used to solve this problem and how they generalize. We first consider the well known algebraic bounds on the independence number, and see how more recent results generalize these existing bounds to bounds on the k-independence number.

3.1 Independent Set and Independence Number

Definition 3.1.1. An *independent set*, also known as a *stable set or coclique*, in a graph is a set of vertices, no two of which are adjacent. The size of a largest independent set, denoted by α, is called the *independence number*.

Let us consider two well-known algebraic bounds on the independence number of a graph, namely, the ratio bound (Hoffman bound) and the inertia bound (Cvetković bound). Though they can be proved by other algebraic means, we will see how they can be proved using the interlacing technique. We now present the inertia bound due to Cvetković.

Theorem 3.1.2. *[23] Suppose that the adjacency matrix of a graph G of order n has eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Assume there are p positive eigenvalues, q negative eigenvalues (counting multiplicities) and the multiplicity of 0 as an eigenvalue is z. Then the size of an independent set is at most $\min\{p+z, q+z\}$. That is,*

$$\alpha(G) \leq |\{i\ : \lambda_i \geq 0\}| \text{ and } \alpha(G) \leq |\{i\ : \lambda_i \leq 0\}|.$$

Proof: We prove this theorem using the interlacing technique. Let A be the adjacency matrix of G, and U an independent set of G with $|U| = \alpha(G)$. Let us partition the vertex set $V(G)$ into U and its complement, that is, $V = U \cup U^c$. Let B be the principal submatrix indexed by U. Then B is the adjacency matrix of $G[U]$, the subgraph of G induced by U. Since $G[U]$ consists of α pairwise non-adjacent vertices, it has eigenvalue 0 of multiplicity α. By principal interlacing (Theorem 2.4.2), the eigenvalues of B interlace the eigenvalues of A. Thus $\lambda_\alpha \geq \mu_\alpha = 0$ and $0 = \mu_1 \geq \lambda_{n-\alpha+1}$. Hence $\alpha(G) \leq |\{i \,|\lambda_i \geq 0\}|$ and $\alpha(G) \leq |\{i \,|\lambda_i \leq 0\}|$. ∎

Next is the ratio bound, also called the Hoffman bound.

Theorem 3.1.3. *[42] Let G be a connected δ-regular graph on n vertices with eigenvalues $\delta = \lambda_1 \geq \cdots \geq \lambda_n$. Then*

$$\alpha(G) \leq n\frac{-\lambda_n}{\lambda_1 - \lambda_n}.$$

Proof: Let U be an independent set in G. Consider the partition $\pi = \{U, U^c\}$ of $V(G)$. Let P be the characteristic matrix of π. Then by Proposition 2.5.4, the quotient matrix B of G with respect to partition π is $B = (P^TP)^{-1}P^TAP$. Then

$$B = \begin{bmatrix} 0 & \delta \\ \frac{\alpha\delta}{n-\alpha} & \frac{\delta(n-2\alpha)}{n-\alpha} \end{bmatrix}.$$

Another way to see B is this. Observe that each vertex in U has all of its δ neighbours in U^c, so there are exactly $\alpha\delta$ edges with one endpoint in U and the other in U^c. Hence a vertex in U^c has on average $\frac{\alpha\delta}{n-\alpha}$ neighbours in U, and has on average $\delta - \frac{\alpha\delta}{n-\alpha}$ neighbours in U^c.

Observe that each row of B sums to δ, hence δ is an eigenvalue with eigenvector $\mathbf{1}$. By the Perron-Frobenius theorem, Theorem 2.2.13, δ is the largest eigenvalue (that is, $\mu_1 = \delta$). Moreover, since $\text{tr}(B)$ is the sum of the eigenvalues of B, and

$$\text{tr}(B) = \frac{\delta(n-2\alpha)}{n-\alpha},$$

we have that the second (and hence the least) eigenvalue of B is $\mu_2 = \frac{\delta(n-2\alpha)}{n-\alpha} - \delta = -\frac{\delta\alpha}{n-\alpha}$. Now by Theorem 2.5.5, the eigenvalues of B interlace the eigenvalues of A hence $\mu_2 = -\frac{\delta\alpha}{n-\alpha} \geq \lambda_n$. Solving this inequality for α, and using $\lambda_1 = \delta$, we obtain the bound. ∎

3.2 The k-Independence Number

In this section, we will see how the results on the independence number generalize to the k-independence number.

Definition 3.2.1. A *k-independent set* in a graph G is a set of vertices of G such that any two vertices in the set are at distance at least $k+1$ in G. The *k-independence number* of a graph G, denoted α_k, is the size of a largest k-independent set in G.

The authors of [1] gave some generalizations on results of the independence number, which were also later improved by Abiad, Coutinho, and Fiol in [2]. These bounds on α_k depend on choosing some polynomial $p(x) \in \mathbb{R}_k[x]$; that is, $p(x)$ is a polynomial of degree at most k with real coefficients. The authors of [2] also gave a bound which generalizes the bound on α_k by Fiol in [29]. In Theorems 3.2.2 and 3.2.3 below, we shall describe their generalization of the Hoffman and the Cvetković bounds. The proofs are based on the interlacing technique described in Theorem 2.4.5.

For the rest of this section, and Chapter 4, let G be a graph on n vertices with adjacency matrix A and eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ such that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. We shall denote the distinct eigenvalues of G as $\theta_0 > \theta_1 > \cdots > \theta_d$. Denote $[2, n] = \{2, 3, 4 \ldots, n\}$, and let $p(x) \in \mathbb{R}_k[x]$. We define the following parameters:

- $W(p) = \max_{u \in V}\{(p(A))_{uu}\}$, where $(p(A))_{uu}$ is the (u, u)-entry of the matrix $p(A)$;
- $w(p) = \min_{u \in V}\{(p(A))_{uu}\}$;
- $\lambda(p) = \min_{i \in [2,n]}\{p(\lambda_i)\}$.

The following is the generalization of the Cvetković bound given in [2].

Theorem 3.2.2. *[2] Let G be a graph on n vertices with adjacency matrix A and eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ such that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Let $p(x) \in \mathbb{R}_k[x]$ with corresponding parameters $W(p)$ and $w(p)$. Then the k-independence number of G satisfies the bound*

$$\alpha_k \leq \min\Big\{|\{i : p(\lambda_i) \geq w(p)\}|,\ |\{i : p(\lambda_i) \leq W(p)|\Big\}.$$

Proof: Let U be a k-independent set of G with $|U| = \alpha_k$. We may assume that the first α_k rows and columns of A correspond to the vertices of U. Let D be the principal submatrix of $p(A)$ obtained using the first α_k rows and columns of $p(A)$. Since $(A^\ell)_{i,j}$ is the number of walks of length ℓ between vertices i and j, we have that $(A^\ell)_{i,j} = 0$ for all $\ell \leq k$ and $i, j \in U, i \neq j$. Hence D is a diagonal matrix. Let $R^T = (\mathbf{I}_{\alpha_k}|\mathbf{0})$ be an $\alpha_k \times n$ matrix. Then $R^T R = I_{\alpha_k}$. Moreover,

$$R^T p(A) R = D.$$

Let $\mu_1 \geq \mu_2 \cdots \geq \mu_{\alpha_k}$ be the eigenvalues of D. Recall that by Lemma 2.2.16, the eigenvalues of $p(A)$ are $p(\lambda_1), \ldots, p(\lambda_n)$. Rename these eigenvalues so that $\zeta_1 \geq \cdots \geq \zeta_n$. Then by Principal Interlacing (Theorem 2.4.2), the eigenvalues of D interlace the eigenvalues of $p(A)$; that is, $\zeta_i \geq \mu_i \geq \zeta_{n-\alpha_k+i}$ for $i = 1, \ldots, \alpha_k$. In particular, $\zeta_{\alpha_k} \geq \mu_{\alpha_k}$, so there must be at least α_k eigenvalues of $p(A)$ larger than or equal to μ_{α_k}. Since $w(p) = \min\{(p(A))_{uu} : u \in V\}$ and $\mu_1, \ldots, \mu_{\alpha_k}$ are α_k of the n diagonal entries of $p(A)$, we have that $w(p) \leq \min\{\mu_1, \ldots, \mu_{\alpha_k}\} = \mu_{\alpha_k}$. Hence

$$\alpha_k \leq |\{i : p(\lambda_i) \geq \mu_{\alpha_k} \geq w(p)\}|.$$

Similarly, as $W(p) = \max\{(p(A))_{uu} : u \in V\}$, we have $W(p) \geq \max\{\mu_1, \ldots, \mu_{\alpha_k}\} = \mu_1$. By interlacing, $\mu_1 \geq \zeta_{n-\alpha_k+1}$, so there must be at least α_k eigenvalues of $p(A)$ smaller than or equal to μ_1. So we have

$$\alpha_k \leq |\{i : p(\lambda_i) \leq \mu_1 \leq W(p)\}|.$$

∎

We now give the Hoffman-like bound.

Theorem 3.2.3. *[2] Let G be a δ-regular graph on n vertices with adjacency matrix A and eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ such that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Let p be any polynomial in $\mathbb{R}_k[x]$ with corresponding parameters $W(p)$ and $\lambda(p)$, and assume $p(\lambda_1) > \lambda(p)$. Then*

$$\alpha_k \leq n\frac{W(p) - \lambda(p)}{p(\lambda_1) - \lambda(p)}. \tag{3.2.1}$$

Proof: Let U be a k-independent set in G with $|U| = \alpha_k = r$. We may assume that the first r rows and columns of A correspond to the vertices of U. Consider the partition $\pi = \{U, U^c\}$ of $V(G)$. Let D be the principal submatrix of $p(A)$ obtained using the first r rows and columns of $p(A)$.

Observe that since $(A^\ell)_{ij}$ is the number of walks of length ℓ between vertices i and j, we have that $(A^\ell)_{ij} = 0$ for all $\ell \leq k$ and $i, j \in U, i \neq j$. Therefore, we can see that D is the diagonal matrix with diagonal entries $(p(A))_{11}, (p(A))_{22} \ldots, (p(A))_{rr}$.

Let B be the quotient matrix of $p(A)$ with respect to π. Recall that B_{ij} is the average row sum of the block $p(A)_{(ij)}$. Since block $p(A)_{(11)} = D$, we have that $B_{11} = \frac{1}{r}\sum_{u\in U}(p(A))_{uu}$. Note that A has each row sum equal to δ, and $\delta = \lambda_1$ by Proposition 2.2.14, so by Lemma 2.2.16, $p(A)$ has each row sum equal to $p(\lambda_1)$. Hence the average row sum of block $p(A)_{(12)}$ is $B_{12} = \frac{rp(\lambda_1) - \sum_{u\in U}(p(A))_{uu}}{r} = p(\lambda_1) - \frac{1}{r}\sum_{u\in U}(p(A))_{uu}$. Observe that $p(A)_{(21)} = p(A)^T_{(12)}$, thus the average row sum of block $p(A)_{(21)}$ is $B_{21} = \frac{rp(\lambda_1) - \sum_{u\in U}(p(A))_{uu}}{n-r}$. Finally, we have $B_{22} = p(\lambda_1) - \frac{rp(\lambda_1) - \sum_{u\in U}(p(A))_{uu}}{n-r}$. Thus the quotient matrix B of $p(A)$ with respect to π is

$$B = \begin{bmatrix} \frac{1}{r}\sum_{u\in U}(p(A))_{uu} & p(\lambda_1) - \frac{1}{r}\sum_{u\in U}(p(A))_{uu} \\ \frac{rp(\lambda_1) - \sum_{u\in U}(p(A))_{uu}}{n-r} & p(\lambda_1) - \frac{rp(\lambda_1) - \sum_{u\in U}(p(A))_{uu}}{n-r} \end{bmatrix} \tag{3.2.2}$$

Each row of B sums to $p(\lambda_1)$, hence B has eigenvector $\mathbf{1}$ with eigenvalue $\mu_1 = p(\lambda_1)$. By Proposition 2.2.14, μ_1 is the largest eigenvalue of B. So the smallest eigenvalue of B will be

$$\mu_2 = \operatorname{tr}(B) - p(\lambda_1) = \frac{1}{r}\sum_{u\in U}(p(A))_{uu} - \frac{rp(\lambda_1) - \sum_{u\in U}(p(A))_{uu}}{n-r}.$$

Recall that by Lemma 2.2.16, the eigenvalues of $p(A)$ are $p(\lambda_1), \dots, p(\lambda_n)$. Rename these eigenvalues so that $\zeta_1 \geq \cdots \geq \zeta_n$ are the eigenvalues of $p(A)$. By Theorem 2.5.5, the eigenvalues of B interlace the eigenvalues of $p(A)$; that is, $\zeta_i \geq \mu_i \geq \zeta_{n-2+i}$ for $i = 1, 2$. In particular, $\mu_2 \geq \zeta_n = \lambda(p)$, which is the least eigenvalue of $p(A)$ by our assumption that $p(\lambda_1) > \lambda(p)$. Since $W(p) = \max\{(p(A))_{uu} : u \in V\}$, we have that $W(p) \geq \frac{1}{r}\sum_{u\in U}(p(A))_{uu}$, the average of $\{(p(A))_{uu} : u \in U\}$.

Hence we have

$$\lambda(p) \leq \mu_2 \leq W(p) - \frac{rp(\lambda_1) - rW(p)}{n-r}. \tag{3.2.3}$$

Rearranging the inequality $\lambda(p) \leq W(p) - \frac{rp(\lambda_1)-rW(p)}{n-r}$, we obtain

$$(p(\lambda_1) - \lambda(p))r \leq n(W(p) - \lambda(p)).$$

Since $p(\lambda_1) - \lambda(p) > 0$, we obtain

$$r \leq n\frac{W(p) - \lambda(p)}{p(\lambda_1) - \lambda(p)}.$$

Hence the result. ∎

Definition 3.2.4. Let G be a regular graph on n vertices with the eigenvalues $\operatorname{ev}(G) = \{\theta_0, \theta_1^{m_1}, \dots, \theta_d^{m_d}\}$, where $\theta_0 > \theta_1 > \cdots > \theta_d$. Let $B(p, \operatorname{ev}(G)) = n\frac{W(p)-\lambda(p)}{p(\theta_0)-\lambda(p)}$. A polynomial $p \in \mathbb{R}_k[x]$, satisfying $p(\theta_0) > \lambda(p)$, is called *optimal* with respect to k if it gives the lowest possible bound for $\alpha_k(G)$ of the form $B(p, \operatorname{ev}(G))$.

Observe that for $c \in \mathbb{R}$, we have $W(p + c) = W(p) + c$, and $W(cp) = cW(p)$. Similarly, $\lambda(p + c) = \lambda(p) + c$ and $\lambda(cp) = c\lambda(p)$. Moreover, $(p + c)(\theta_0) = p(\theta_0) + c$ and $(cp)(\theta_0) = cp(\theta_0)$. Thus, an optimal polynomial $p(x) \in \mathbb{R}_k[x]$ can be taken to be monic and without a constant term. We shall simply write the expression $B(p, \operatorname{ev}(G))$ as $B(p)$ if there is no ambiguity.

For $k = 1$, any linear polynomial satisfying $p(\lambda_1) \geq \lambda(p)$ is optimal. We can let $p(x) = x$. Then $W(p) = 0, p(\lambda_1) = \lambda_1, \lambda(p) = p(\lambda_n) = \lambda_n$, and so (3.2.1) gives the Hoffman bound

$$\alpha_1 = \alpha \leq n\frac{-\lambda_n}{\lambda_1 - \lambda_n}. \tag{3.2.4}$$

The authors in [2] gave an optimal polynomial for $k = 2$.

Corollary 3.2.5. *[2] Let G be a δ-regular graph on n vertices, with adjacency matrix A. Assume that all the distinct eigenvalues of G are $\delta = \theta_0 > \theta_1 > \cdots > \theta_d$, with $d \geq 2$, and that θ_i is the largest eigenvalue such that $\theta_i \leq -1$. Then $p(x) = x^2 - (\theta_i + \theta_{i-1})x$ is an optimal polynomial for $k = 2$, and the corresponding bound on α_2 is*

$$\alpha_2 \leq n \frac{\theta_0 + \theta_i \theta_{i-1}}{(\theta_0 - \theta_i)(\theta_0 - \theta_{i-1})}. \tag{3.2.5}$$

Proof: To show that the right hand side in (3.2.5) is indeed $B(p)$, recall that $(A^k)_{uu}$ is the number of closed walks of length k centred at vertex u, and so $(A^2)_{uu} = \delta = \theta_0$ and $(A)_{uu} = 0$. Hence

$$W(p) = \max_{u \in V}\{(p(A))_{uu}\} = \max_{u \in V}\{(A^2)_{uu} - (\theta_i + \theta_{i-1})(A)_{uu}\} = \theta_0 - (\theta_i + \theta_{i-1})(0) = \theta_0.$$

As $p(x)$ attains its global minimum at $x = \frac{\theta_i + \theta_{i-1}}{2}$, and $p(\theta_i) = p(\theta_{i-1})$, we have $\lambda(p) = p(\theta_i) = p(\theta_{i-1}) = -\theta_i\theta_{i-1}$. Finally, $p(\theta_0) = \theta_0^2 - (\theta_i + \theta_{i-1})\theta_0$. So using these details in the expression for $B(p)$ in Theorem 3.2.3, we obtain the bound (3.2.5).

We now present details of the proof of optimality of $p(x) = x^2 - (\theta_i + \theta_{i-1})x$ as was given in [2]. Let $p(x) = ax^2 + bx + c$ and suppose first that $a > 0$. Then, from the expression of the bound in (3.2.1), there is no loss of generality if we take $a = 1$ and $c = 0$. Then, the minimum of the polynomial $p(x) = x^2 + bx$ is attained at $x = -b/2$ and, hence, given b, the minimum $\lambda(p)$ must be equal to $p(\theta_i)$ where θ_i is the eigenvalue closest to $-b/2$. Now we proceed to find the optimal value for b. If $\theta_i \neq \theta_d$, from $(\theta_i + \theta_{i+1})/2 \leq -b/2 \leq (\theta_i + \theta_{i-1})/2$ we can write that $b = -\theta_i + \tau$ for $\tau \in [-\theta_{i-1}, -\theta_{i+1}]$. Otherwise, if $i = d$, from $-b/2 \leq (\theta_d + \theta_{d-1})/2$, we get that $b = -\theta_d + \tau$ with $\tau \geq -\theta_{d-1}$. Then, in both cases, we have $W(p) = \theta_0$, $\lambda(p) = p(\theta_i) = \tau\theta_i$, and $p(\theta_0) = \theta_0^2 + (-\theta_i + \tau)\theta_0$. Observe that $p(\theta_0) > \lambda(p)$. The bound in (3.2.1), as a function of τ , is

$$\varPhi(\tau) = n \frac{\theta_0 - \theta_i \tau}{(\theta_0 - \theta_i)(\theta_0 + \tau)},$$

with derivative $\varPhi(\tau)' = n \frac{-\theta_0(1+\theta_i)}{(\theta_0 - \theta_i)(\theta_0 + \tau)^2}$. Consequently, the resulting bound $\varPhi(\tau)$ is an increasing, constant, or decreasing function depending on $\theta_i < -1$, $\theta_i = -1$, or $\theta_i > -1$, respectively. Since we are interested in the minimum value of $\varPhi$, we reason as follows:

- If $\theta_i < -1$, we must take the value of τ as small as possible, that is $\tau = -\theta_{i-1}$, which gives $\alpha_2 \leq \varPhi(-\theta_{i-1}) = n \frac{\theta_0 + \theta_i \theta_{i-1}}{(\theta_0 - \theta_i)(\theta_0 - \theta_{i-1})}$. Moreover, iterating the reasoning, we eventually take for θ_i the largest eigenvalue smaller than -1, as claimed.

- If $\theta_i = -1$ we have that $\theta_{i+1} > -1$ and, with θ_i taking the role of θ_{i+1}, we are in the next case.

- If $\theta_i > -1$, we must take the value of τ as large as possible, that is $\tau = -\theta_{i+1}$, which gives $\alpha_2 \leq \Phi(-\theta_{i+1}) = n\frac{\theta_0+\theta_i\theta_{i+1}}{(\theta_0-\theta_i)(\theta_0-\theta_{i+1})}$. Again, iterating the procedure, we eventually take for θ_i the smallest eigenvalue greater than -1, as claimed. Moreover, θ_{i+1} is the largest eigenvalue that is at most -1, in agreement with our claim.

To show that the polynomial p is best possible, we assume now that $a < 0$ and, then, we reason with $p(x) = -x^2 + bx$. First, to satisfy the condition $p(\theta_0) > \lambda(p)$, we must have $b > \theta_0 + \theta_d$. Then, $\lambda(p) = p(\theta_d) = -\theta_d^2 - b\theta_d$ and the bound in (3.2.1) as a function of b, is

$$\Phi(b) = n\frac{-\theta_0 + \theta_d^2 - b\theta_d}{-\theta_0^2 + \theta_d^2 + b(\theta_0 - \theta_d)},$$

which is decreasing for $b > \theta_0 + \theta_d$. Then, we should take $\lim_{b\to\infty} \Phi(b) = n\frac{-\theta_d}{\theta_0-\theta_d}$. But this is again the Hoffman's bound in (3.2.4) for α_1, which clearly holds for α_2. ∎

For a general k, the authors of [2] use the polynomial $p(x) = \sum_{j=1}^{k} x^j$ to obtain a bound on α_k of the form (3.2.1). For this $p(x)$, we have $W(p) = \max_{u\in V}\{\sum_{j=1}^{k}(A^k)_{uu}\}$. Then, the k-independence number of G satisfies the following.

i. If k is odd, then $p(x)$ is strictly increasing. This can be seen by observing that the derivative $p'(x)$ can be written as $p'(x) = \sum_{i=1}^{(k-1)/2} i(x^{i-1} + x^i)^2 + \frac{k+1}{2}x^{k-1}$, which is a sum of only non-negative terms. So $\lambda(p) = p(\theta_d)$. Hence we have

$$\alpha_k \leq n\frac{W(p) - \sum_{j=1}^{k}\theta_d^j}{\sum_{j=1}^{k}\theta_0^j - \sum_{j=1}^{k}\theta_d^j}. \tag{3.2.6}$$

ii. If k is even, then $p(x)$ has minimum value approaching $-\frac{1}{2}$ as $k \to \infty$, which is shown to imply

$$\alpha_k \leq n\frac{W(p) + 1/2}{\sum_{j=1}^{k}\theta_0^j + 1/2}. \tag{3.2.7}$$

The next result is due to Fiol and it requires a preliminary definition.

Definition 3.2.6. Let $G = (V, E)$ be a graph with adjacency matrix A with the eigenvalues $\mathrm{ev}(G) = \{\theta_0, \theta_1^{m_1}, \ldots, \theta_d^{m_d}\}$. For a given $k = 0, 1, \ldots, d$, let us consider the set of real polynomials $P_k = \{f \in \mathbb{R}_k[x] : f(\theta_0) = 1, f(\theta_i) \geq 0, \text{ for } 1 \leq i \leq d\}$, and the continuous function $\Psi : P_k \to \mathbb{R}^+$ defined by $\Psi(f) = \operatorname{tr} f(A)$. Then, the *$k$-minor polynomial* of G is the polynomial f_k at which Ψ attains its minimum:

$$\operatorname{tr} f_k(A) = \min\{\operatorname{tr} f(A) : f \in P_k\}. \tag{3.2.8}$$

A graph is called *k-partially walk-regular* if the number of closed walks of a given length $l \leq k$, rooted at a vertex v, only depends on l. We now state the result by Fiol [31].

Theorem 3.2.7. *(Fiol [31]) Let G be a k-partially walk-regular graph with n vertices, adjacency matrix A, and the eigenvalues $\mathrm{ev}(G) = \{\theta_0, \theta_1^{m_1}, \ldots, \theta_d^{m_d}\}$. Let $f_k \in \mathbb{R}_k[x]$ be a k-minor polynomial. Then, for every $k = 0, \ldots, d-1$, the k-independence number α_k of G satisfies*

$$\alpha_k \leq \mathrm{tr}\, f_k(A) = \sum_{i=0}^{d} m_i f_k(\theta_i). \tag{3.2.9}$$

So, in some sense, a k-minor polynomial of G is an optimal polynomial for $\alpha_k(G)$. As a consequence of Theorem 3.2.7, it was shown by Fiol [31] that for the case $k = 1$, which coincides with the standard independence number, the minor polynomial is $f_i = \frac{x-\theta_d}{\theta_0-\theta_d}$. Moreover, the bound on α_1 coincides with the Hoffman bound in Theorem 3.1.3. Moreover, for the case $k = 2$, the minor polynomial is $f_2 = \frac{(x-\theta_i)(x-\theta_{i-1})}{(\theta_0-\theta_i)(\theta_0-\theta_{i-1})}$, where θ_i is the largest eigenvalue not greater than -1 and α_2 is in agreement with Corollary 3.2.5. In the general case, $1 \leq k \leq d$, the following was obtained.

Theorem 3.2.8. *(Fiol [31]) Let $I \subset \{1, \ldots, d\}$ range over all index sets with k elements (and if k is odd, it can be required that $d \in I$). Then,*

$$\alpha_k \leq \mathrm{tr}\, f_k(A) = \min_I \sum_{j \notin I} m_j \prod_{i \in I} \frac{\theta_j - \theta_i}{\theta_0 - \theta_i}. \tag{3.2.10}$$

For the case $k = 3$ in particular, Fiol proposed the minor polynomial $f_3 = f_1 f_2$ as good (and often optimal) choice. With this choice of polynomial we have the following.

Corollary 3.2.9. (Fiol [31]) If G is at least 3-partially walk-regular, and n_t is the common number of triangles rooted at every vertex of G, then

$$\alpha_3 \leq \mathrm{tr}\, f_3 = n \frac{2n_t - \theta_0(\theta_d + \theta_i + \theta_{i-1}) - \theta_d \theta_i \theta_{i-1}}{(\theta_0 - \theta_d)(\theta_0 - \theta_i)(\theta_0 - \theta_{i-1})}, \tag{3.2.11}$$

where θ_i is the largest eigenvalue not greater than -1.

Our overarching objective is to derive an optimal polynomial for $k \geq 3$. In the upcoming chapter, we specifically focus on the case $k = 3$. We demonstrate that the bound given in (3.2.6) for $k = 3$ is not optimal. Furthermore, we conduct a comparative analysis between Fiol's bound, as stated in Corollary 3.2.9, and the bound resulting from our polynomial. Our findings reveal that our bound is the best achievable, and we elucidate instances where Fiol's bound coincides with ours. It is noteworthy that our discovery of Fiol's bound occurred after the formulation of our results.

Chapter 4

The Optimal Bound on the 3-Independence Number

In this chapter, we present the optimal bound on the 3-independence number obtainable using a polynomial.

4.1 Towards an Optimal Polynomial for $k = 3$

Let G be a δ-regular graph with n vertices and adjacency matrix A. Assume that all the distinct eigenvalues of G are $\delta = \theta_0 > \theta_1 > \cdots > \theta_d$, with $d \geq 3$. Using the definitions from Chapter 3, let p be any polynomial in $\mathbb{R}_3[x]$ with corresponding parameters $W(p)$ and $\lambda(p)$, and assume $p(\lambda_1) > \lambda(p)$. Our goal in this section is to get an optimal polynomial for $k = 3$. Recall that Abiad. et al. [2] proposed the polynomial $p(x) = \sum_{j=1}^{k} x^j$ for arbitrary k. In what follows, we show that it is not optimal for $k = 3$.

Proposition 4.1.1. *The polynomial $f(x) = x^3 + x^2 + x \in \mathbb{R}_3[x]$ is not optimal with respect to $k = 3$.*

Proof: We prove the claim by showing that for graphs with girth greater than three, the polynomial $p(x) = x^3 + x^2$ gives a better bound than $f(x) = x^3 + x^2 + x$. Since the graph has girth greater than 3, we know $(A^3)_{uu} = 0$. So we have $W(f) = \max_{u \in V}\{(f(A))_{uu}\} = \max_{u \in V}\{(A^3)_{uu} + (A^2)_{uu} + (A)_{uu}\} = 0 + \delta + 0 = \theta_0$. Similarly, $W(p) = \theta_0$. Since $f(x)$ is an increasing function, we know that $\lambda(f) = f(\theta_d)$, so using $f(x)$ in the expression for $B(f)$ in Inequality (3.2.6) we get

$$B(f) = n\frac{\theta_0 - (\theta_d^3 + \theta_d^2 + \theta_d)}{(\theta_0^3 + \theta_0^2 + \theta_0) - (\theta_d^3 + \theta_d^2 + \theta_d)}. \tag{4.1.1}$$

On the other hand, $p(x)$ is strictly increasing on the intervals $(-\infty, \frac{-2}{3}) \cup (0, \infty)$, and intercepts the x-axis at $x = -1$ and $x = 0$. Since $\theta_d \leq -1$ by Lemma 2.4.4, we have

$\lambda(p) = p(\theta_d)$. So using $p(x)$ in the expression for $B(p)$ in Theorem 3.2.3 we have the bound

$$B(p) = n\frac{\theta_0 - (\theta_d^3 + \theta_d^2)}{(\theta_0^3 + \theta_0^2) - (\theta_d^3 + \theta_d^2)}. \tag{4.1.2}$$

We show that $B(p) < B(f)$ for these graphs. Let us determine when $B(f) < B(p)$, that is, when

$$\frac{\theta_0 - (\theta_d^3 + \theta_d^2 + \theta_d)}{(\theta_0^3 + \theta_0^2 + \theta_0) - (\theta_d^3 + \theta_d^2 + \theta_d)} < \frac{\theta_0 - (\theta_d^3 + \theta_d^2)}{(\theta_0^3 + \theta_0^2) - (\theta_d^3 + \theta_d^2)}.$$

This inequality is equivalent to

$$-\theta_d\theta_0^3 - (\theta_d + 1)\theta_0^2 + (\theta_d + \theta_d^2 + \theta_d^3)\theta_0 < 0. \tag{4.1.3}$$

We solve Inequality (4.1.3) for θ_0 in terms of θ_d. Let

$$h(\theta_0) = -\theta_d\theta_0^3 - (\theta_d + 1)\theta_0^2 + (\theta_d + \theta_d^2 + \theta_d^3)\theta_0 = 0. \tag{4.1.4}$$

Observe that θ_d and 0 are roots of $h(\theta_0)$, and the third root is a positive number, call it μ. So we have that $B(f) < B(p)$ if and only if $0 < \theta_0 < \mu$. Since $h(-\theta_d) = -2\theta_d(\theta_d^2 + \theta_d) > 0$, we can deduce that $\mu < -\theta_d$. But $-\theta_d \leq \theta_0$ by Theorem 2.2.13. Hence $\mu < \theta_0$ and so $B(f) > B(p)$. Thus the polynomial $p(x) = x^3 + x^2$ gives a better bound than $f(x) = x^3 + x^2 + x$ for graphs of girth greater than 3. ∎

4.2 The Polynomial of the Form $p(x) = x^3 + bx^2 + cx$

In this section, we present an optimal polynomial for $k = 3$, thereby establishing an optimal bound for α_3 among all bounds of the form given in Theorem 3.2.3. The following lemma will be instrumental in our derivation.

If we consider $p(x) = x^3 + bx^2 + cx$ and set $x = \theta_i$, and let c vary, we get a linear function $p_i(c) = \theta_i^3 + b\theta_i^2 + c\theta_i$ of slope θ_i. Since $\theta_d < \theta_i$ for all $i \neq d$ then for c sufficiently large enough, $p_d(c) < p_i(c)$ and for c small $p_d(c) > p_i(c)$.

Lemma 4.2.1. *Let $d \geq 3$, and $\theta_0, \theta_1, \ldots, \theta_d$ be real numbers with $\theta_0 > \cdots > \theta_d$. Consider $b \in \mathbb{R}$ fixed throughout. Let $p(x) = x^3 + bx^2 + cx$, where $c \in \mathbb{R}$. For $i = 0, 1, \ldots, d$, let $p_i(c) = p(\theta_i)$ and $\lambda(p) = \min\{p_i(c) : i = 1, \ldots, d\}$. Let c^* be the largest value of c such that $p_d(c) = p_i(c)$ for some value of i, and denote such i as j. Let $c = c_i^*$ be the solution of the linear equation $p_i(c) = p_{i-1}(c)$ for $i = 1, 2, \ldots, j$. Define the intervals*

$$I_s = [c_s^*, c_{s+1}^*] \text{ for } s = 1, \ldots, j-1, \quad I_j = [c_j^*, c^*], \text{ and } I_d = [c^*, \infty).$$

Then, $\lambda(p) = p(\theta_i)$ if $c \in I_i$ for $i \in \{1, \ldots, j\} \cup \{d\}$.

Proof: Let $\Lambda = \{\theta_0, \ldots, \theta_d\}$, so $\lambda(p) = \min\{p(x) : x \in \Lambda \backslash (\theta_0)\}$.

If we differentiate $p(x)$, we observe that it has a local maximum at $x_1 = \frac{1}{3}(-b - \sqrt{b^2 - 3c})$ and a local minimum at $x_2 = \frac{1}{3}(-b + \sqrt{b^2 - 3c})$ if $c < \frac{b^2}{3}$. If $c \geq \frac{b^2}{3}$, then $p(x)$ is increasing and has no turning point and hence, on $[\theta_d, \infty]$ it attains an absolute minimum at θ_d. Thus, we have $\lambda(p) = p(\theta_d)$ if $c \geq \frac{b^2}{3}$.

So, for $c < \frac{b^2}{3}$, we have that on $[\theta_d, \infty)$, $p(x)$ attains an absolute minimum at x_2 or at θ_d. We explore this case further.

Consider x_2 as a function of c; that is, $x_2(c) = \frac{1}{3}(-b + \sqrt{b^2 - 3c})$. Observe that $x_2(c)$ is continuous and decreasing on $(-\infty, \frac{b^2}{3})$, with $\lim_{c \to \frac{b^2}{3}} x_2(c) = \frac{-b}{3}$ and $\lim_{c \to -\infty} x_2(c) = \infty$. So, as c increases, the local minimum occurs at smaller values of x_2. Let m be the maximum index such that $\theta_m > \frac{-b}{3}$. Then, over Λ, for $i = 0, 1, \ldots, m$, there exists $c_i \in (-\infty, \frac{b^2}{3})$ such that $x_2(c_i) = \theta_i$, and $c_0 < c_1 < \cdots < c_m$. That is, if $c = c_i$, then $x_2 = \theta_i$ and absolute minimum of $p(x)$ occurs at $x = \theta_i$ or $x = \theta_d$.

Now, for $i \in \{1, \ldots, m\}$, let c_i^* be the c coordinate of intersection of $p_i(c)$ and $p_{i-1}(c)$ and define $\Upsilon(c) = \min\{p_i(c)\}$. Then $\Upsilon(c)$ is a concave down piece-wise linear function. Since $c_0 < c_1 < \cdots < c_m$ and $c_{i-1} < c_i^* < c_i$, we have $c_1^* < c_2^* < \cdots < c_m^* < c_m$. Now since $\theta_i < \theta_{i-1}$, if $c \geq c_i^*$ then $p_i(c) < p_{i-1}(c) < \cdots < p_1(c)$. Similarly, if $c \leq c_{i+1}^*$ then $p_i(c) < p_{i+1}(c) < \cdots < p_m(c)$. Hence, $\Upsilon(c) = p_i(c)$ if $c \in [c_i^*, c_{i+1}^*]$. Observe that, at $c = \frac{b^2}{3}$, we have $p_d(c) < p_m(c) < p_{m-1}(c) < \cdots < p_1(c)$. Hence, line $p_d(c)$, having the least slope, intersects $\Upsilon(c)$ at some point say, $(c^*, \Upsilon(c^*))$. Then, c^* is the largest value of c such that $p_d(c) = p_i(c)$ for some value of i. Thus, $p_d(c) \leq \Upsilon(c)$ for $c \in [c^*, \frac{b^2}{3})$

Hence, for the largest $j \in \{1, \ldots, m\}$ such that $c_j^* < c^*$, we have $c_1^* < c_2^* < \cdots < c_j^* < c^*$, and so

$$\lambda(p) = \begin{cases} p_s(c), & \text{if } c_s^* \leq c \leq c_{s+1}^* \text{ for all } 1 \leq s \leq j-1, \\ p_j(c), & \text{if } c_j^* \leq c \leq c^*, \\ p_d(c), & \text{if } c^* \leq c < \infty. \end{cases}$$

∎

We now present our main result.

Theorem 4.2.2. *Let G be a δ-regular graph with n vertices, adjacency matrix A, and distinct eigenvalues $\delta = \theta_0 > \theta_1 > \cdots > \theta_d$, with $d \geq 3$. Let s be the largest index such that $\theta_s \geq -\frac{\theta_0^2 + \theta_0\theta_d - \triangle}{\theta_0(\theta_d + 1)}$, where $\triangle = max_{u \in V}\{(A^3)_{uu}\}$. Let $b = -(\theta_s + \theta_{s+1} + \theta_d)$ and $c = \theta_d\theta_s + \theta_d\theta_{s+1} + \theta_s\theta_{s+1}$. Then, $p(x) = x^3 + bx^2 + cx$ is an optimal polynomial for $k = 3$. The corresponding bound on the 3-independence number of G is*

$$\alpha_3 \leq n \frac{\triangle - \theta_0(\theta_s + \theta_{s+1} + \theta_d) - \theta_s\theta_{s+1}\theta_d}{(\theta_0 - \theta_s)(\theta_0 - \theta_{s+1})(\theta_0 - \theta_d)}. \tag{4.2.1}$$

If equality is attained, then the matrix $A^3-(\theta_s+\theta_{s+1}+\theta_d)A^2+(\theta_d\theta_s+\theta_d\theta_{s+1}+\theta_s\theta_{s+1})A$ *has a regular partition (with a set of* α_3 *3-independent vertices and its complement) with quotient matrix*

$$B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}, \tag{4.2.2}$$

where

$$\begin{aligned}
B_{11} &= \triangle - (\theta_s + \theta_{s+1} + \theta_d)\delta, \\
B_{12} &= \delta^3 - (\theta_s + \theta_{s+1} + \theta_d)\delta^2 + (\theta_d\theta_s + \theta_d\theta_{s+1} + \theta_s\theta_{s+1} + \theta_s + \theta_{s+1} + \theta_d)\delta - \triangle, \\
B_{21} &= \triangle - (\theta_s + \theta_{s+1} + \theta_d)\delta - \theta_s\theta_{s+1}\theta_d, \\
B_{22} &= \delta^3 - (\theta_s + \theta_{s+1} + \theta_d)\delta^2 + (\theta_d\theta_s + \theta_d\theta_{s+1} + \theta_s\theta_{s+1} + \theta_s + \theta_{s+1} + \theta_d)\delta + \theta_s\theta_{s+1}\theta_d - \triangle.
\end{aligned}$$

If we assume G is at least 3-partially walk-regular, and let n_t be the common number of triangles rooted at every vertex of G, then $\triangle = 2n_t$ and so

$$\alpha_3 \le n\frac{2n_t - \theta_0(\theta_s + \theta_{s+1} + \theta_d) - \theta_s\theta_{s+1}\theta_d}{(\theta_0 - \theta_s)(\theta_0 - \theta_{s+1})(\theta_0 - \theta_d)}, \tag{4.2.3}$$

which is consistent with Fiol's bound in Corollary 3.2.9 if its index i coincides with index $s+1$, otherwise our bound is stronger. We will revisit this in Section 5.7.

In particular, if G is a bipartite graph, then since $\theta_d = -\theta_0$ and $\triangle = 0$, we have that θ_s is the least eigenvalue greater or equal to 0, and the corresponding bound on α_3 in (4.2.1) becomes

$$\alpha_3 \le \frac{\theta_0 - (\theta_s + \theta_{s+1}) + \theta_s\theta_{s+1}}{2(\theta_0 - \theta_s)(\theta_0 - \theta_{s+1})}. \tag{4.2.4}$$

We now prove Theorem 4.2.2.

Proof: Take any $b, c \in \mathbb{R}$, and define a polynomial $p(x) = x^3 + bx^2 + cx$. We show that b and c as stated in the theorem give an optimal polynomial. Assume $\lambda(p)$ occurs at θ_t. Then, $W(p) = \triangle + b\,\theta_0$. Thus, the bound in Equation (3.2.1) becomes

$$\Phi_t(b,c) = \Phi(\theta_t, b, c) = n\frac{\triangle + b\theta_0 - p(\theta_t)}{p(\theta_0) - p(\theta_t)} = n\frac{\triangle + b\theta_0 - (\theta_t^3 + b\theta_t^2 + c\theta_t)}{\theta_0^3 + b\theta_0^2 + c\theta_0 - (\theta_t^3 + b\theta_t^2 + c\theta_t)}. \tag{4.2.5}$$

We investigate the pairs (b, c) that minimize the bound $\Phi_t(b, c)$.

Let $b \in \mathbb{R}$ be fixed. Differentiating (4.2.5) with respect to c gives

$$\begin{aligned}
\frac{\partial}{\partial c}\Phi_t(b,c) &= n\frac{\theta_0\theta_t^3 + b\theta_0\theta_t^2 + (-b\theta_0^2 - \theta_0^3 + b\theta_0 + \triangle)\theta_t - b\theta_0^2 - \theta_0\triangle}{\left[\theta_0^3 + b\theta_0^2 + c\theta_0 - (\theta_t^3 + b\theta_t^2 + c\theta_t)\right]^2} \\
&= n\frac{(\theta_0 - \theta_t)(-b\theta_0\theta_t - \theta_0^2\theta_t - \theta_0\theta_t^2 - b\theta_0 - \triangle)}{(\theta_0 - \theta_t)^2(b\theta_0 + \theta_0^2 + b\theta_t + \theta_0\theta_t + \theta_t^2 + c)^2}
\end{aligned}$$

$$= -n\frac{\theta_0\theta_t^2 + (b\theta_0 + \theta_0^2)\theta_t + (b\theta_0 + \triangle)}{(\theta_0 - \theta_t)(b\theta_0 + \theta_0^2 + b\theta_t + \theta_0\theta_t + \theta_t^2 + c)^2}.$$

The denominator is equal to $(p(\theta_0)-p(\theta_t))^2$ divided by $\theta_0-\theta_t$. Since $p(\theta_0)-p(\theta_t) > 0$ and $\theta_0 - \theta_t > 0$, the denominator is positive. The numerator is a quadratic function in $x = \theta_t$, that is, $f(x) = \theta_0 x^2 + (b\theta_0 + \theta_0^2)x + (b\theta_0 + \triangle)$ with roots

$$x_{1,2} = -\frac{b+\theta_0}{2} \pm \sqrt{\left(\frac{b+\theta_0}{2}\right)^2 - b - \frac{\triangle}{\theta_0}}.$$

Let $\nu = -\frac{b+\theta_0}{2} - \sqrt{\left(\frac{b+\theta_0}{2}\right)^2 - b - \frac{\triangle}{\theta_0}}$ and $\mu = -\frac{b+\theta_0}{2} + \sqrt{\left(\frac{b+\theta_0}{2}\right)^2 - b - \frac{\triangle}{\theta_0}}$.

Since each vertex of G can be on at most $\binom{\theta_0}{2}$ different triangles, we have $\triangle \leq \theta_0(\theta_0 - 1)$. So, we have

$$\begin{aligned}
\left(\frac{b+\theta_0}{2}\right)^2 - b - \frac{\triangle}{\theta_0} &\geq \left(\frac{b+\theta_0}{2}\right)^2 - b - \frac{\theta_0(\theta_0-1)}{\theta_0} \\
&= \left(\frac{b+\theta_0}{2}\right)^2 - b - (\theta_0 - 1) = \left(\frac{b+\theta_0}{2}\right)^2 - (b+\theta_0) + 1 \\
&= \left(\frac{b+\theta_0}{2} - 1\right)^2 \geq 0.
\end{aligned}$$

Thus, ν and μ are real numbers, and

- $\Phi_t(b,c)$ is increasing with respect to c if $\nu < \theta_t < \mu$,
- $\Phi_t(b,c)$ is decreasing with respect to c if $\theta_t < \nu$ or $\theta_t > \mu$,
- $\Phi_t(b,c)$ is constant with respect to c if $\theta_t = \nu$ or $\theta_t = \mu$.

Now we show $\nu \leq -1 \leq \mu$.

$$\begin{aligned}
\mu &= -\frac{b+\theta_0}{2} + \sqrt{\left(\frac{b+\theta_0}{2}\right)^2 - b - \frac{\triangle}{\theta_0}} \\
&\geq -\frac{b+\theta_0}{2} + \sqrt{\left(\frac{b+\theta_0}{2} - 1\right)^2} \\
&= -\frac{b+\theta_0}{2} + \left|\frac{b+\theta_0}{2} - 1\right| \\
&= \begin{cases} -\frac{b+\theta_0}{2} + (-(\frac{b+\theta_0}{2} - 1)) & \text{if } b \leq 2 - \theta_0 \\ -\frac{b+\theta_0}{2} + (\frac{b+\theta_0}{2} - 1) & \text{if } b \geq 2 - \theta_0 \end{cases}
\end{aligned}$$

$$= \begin{cases} -(b+\theta_0)+1 \geq -1 & \text{if } b \leq 2-\theta_0 \\ -1 & \text{if } b \geq 2-\theta_0 \end{cases}.$$

Hence, we have $\mu \geq -1$.

Also, we have

$$\begin{aligned} \nu &= -\frac{b+\theta_0}{2} - \sqrt{\left(\frac{b+\theta_0}{2}\right)^2 - b - \frac{\triangle}{\theta_0}} \\ &\leq -\frac{b+\theta_0}{2} - \sqrt{\left(\frac{b+\theta_0}{2} - 1\right)^2} \\ &= -\frac{b+\theta_0}{2} - \left|\frac{b+\theta_0}{2} - 1\right| \\ &= \begin{cases} -\frac{b+\theta_0}{2} - (-(\frac{b+\theta_0}{2} - 1)) & \text{if } b \leq 2-\theta_0 \\ -\frac{b+\theta_0}{2} - (\frac{b+\theta_0}{2} - 1) & \text{if } b \geq 2-\theta_0 \end{cases} \\ &= \begin{cases} -1 & \text{if } b \leq 2-\theta_0 \\ -(b+\theta_0)+1 \leq -1 & \text{if } b \geq 2-\theta_0 \end{cases}. \end{aligned}$$

Thus, we have $\nu \leq -1$.

Now, for a fixed b, we determine an optimal c, that is, a c that will minimize $\Phi_t(b,c)$.

Adopt the notation of Lemma 4.2.1, and let $p_i(c) = p(\theta_i)$ and $\lambda(p) = \min\{p_i(c) : i = 1, \ldots, d\}$, we define the intervals

$$I_\ell = [c_\ell, c_{\ell+1}] \text{ for } \ell = 1, \ldots, j-1,\ I_j = [c_j, c^*],\ \text{and } I_d = [c^*, \infty).$$

Recall that c^* is the largest value of c such that $p_d(c) = p_i(c)$ for some value of i denoted as j, and $c = c_i$ is the solution of the linear equation $p_i(c) = p_{i-1}(c)$ for $i = 1, \ldots, j$. Recall also that by Lemma 4.2.1, if $c \in I_i$, then $\lambda(p) = p(\theta_i)$, that is, θ_i minimizes p. Observe that, by choosing any $c \in I_i$ for $i \in \{1, \ldots, j\} \cup \{d\}$, we ensured $p(\theta_0) > \lambda(p)$. Note that, for b fixed, we aim to find $\Omega = \min\{\Phi_i(b,c) : i \in \{1, 2, \ldots, j, d\}, c \in I_i\}$. As $\lambda(p)$ is constant and $\Phi_i(b,c)$ is monotone on each of the intervals $I_1, \ldots, I_j, I_d$, we only need to compare the values of $\Phi_i(b,c)$ at interval endpoints. In particular, since $\nu \leq -1 \leq \mu$, we observe the following.

Let i' be such that $\theta_{i'}$ is the largest eigenvalue with $\theta_{i'} \leq \mu$, and let j' be such that $\theta_{j'}$ is the largest eigenvalue with $\theta_{j'} \leq \nu$.

Case 1. If $\theta_i \leq \nu$. In this case, $\Phi_i(b,c)$ is decreasing or constant on I_i. Hence, if $i \neq d$, then the minimum of $\Phi_i(b,c)$ exists and is attained at the right endpoint of the interval, that is, at

$$\begin{cases} c_{i+1} & \text{if } j' \leq i \leq j-1, \\ c^* & \text{if } i = j. \end{cases}$$

In particular, we have

$$\Phi_m(b, c_{m+1}) = \Phi_{m+1}(b, c_{m+1}) \geq \Phi_{m+1}(b, c_{m+2}) \text{ for all } j' \leq m \leq j-1,$$

and

$$\Phi_{j-1}(b, c_j) = \Phi_j(b, c_j) \geq \Phi_j(b, c^*) = \Phi_d(b, c^*) \geq \Phi_d(b, c) \text{ for all } c > c^*.$$

Thus, we have

$$\Omega = \min\{\Phi_i(b,c) : i \in \{j', j'+1, \ldots, j, d\}, c \in I_i\} = \Phi_d(b,c) \text{ for all } c > c^*.$$

However, $\Phi_d(b,c)$ has no minimum on I_d but $\lim_{c\to\infty} \Phi_d(b,c) = n\frac{-\theta_d}{\theta_0-\theta_d}$ is an upper bound on α_3 and it is less than any other bound in this case. But this is the Hoffman bound for α_1, which clearly holds for α_3.

Case 2. If $\mu < \theta_i$. In this case, $\Phi_i(b,c)$ is decreasing on I_i. Hence, $\Phi_i(b,c)$ attains its minimum at the right endpoint of I_i; that is, at c_{i+1} for $1 < i \leq i'-1$. Recall that $\theta_{i'-1}$ is the smallest eigenvalue greater than μ. In particular, the minimum occurs at

$$\begin{cases} c_{i+1} & \text{if } 1 \leq i \leq j-1, \\ c^* & \text{if } i = j. \end{cases}$$

We observe the following. If $m \in \{1, \ldots i'-1\}$, then

$$\Phi_m(b, c_{m+1}) = \Phi_{m+1}(b, c_{m+1}) > \Phi_{m+1}(b, c_{m+2}) \text{ for all } 1 \leq m \leq i'-1.$$

Thus, we have

$$\Omega = \min\{\Phi_i(b,c) : i \in \{1, \ldots, i'-1\}, c \in I_i\} = \Phi_{i'-1}(b, c_{i'}).$$

Note that $j > i'-1$ or $j \leq i'-1$. Thus, we have two possibilities here, that is, either $\theta_j < \mu$ or $\theta_j \geq \mu$. In particular,

$$\Omega = \begin{cases} \Phi_{i'-1}(b, c_{i'}) & \text{if } j \geq i', \\ \Phi_j(b, c^*) & \text{if } j < i'. \end{cases}$$

That is, for all i such that $\mu < \theta_i$, the bound $\Phi_i(b,c)$ is minimized at $i = i'-1$ with $c = c_{i'}$ if $j \geq i'$, or at $i = j$ with $c = c^*$ if $j \leq i'-1$.

Case 3. If $\nu \leq \theta_i \leq \mu$. In this case, $\Phi_i(b,c)$ is increasing or constant on I_i. Hence, $\Phi_i(b,c)$ attains its minimum at the left endpoint of I_i; that is, at

$$\begin{cases} c_i & \text{if } i' \leq i \leq j, \\ c^* & \text{if } i = d. \end{cases}$$

Now we have that $\Phi_d(b,c^*) = \Phi_j(b,c^*) \geq \Phi_j(b,c_j)$. Moreover,

$$\Phi_m(b,c_m) = \Phi_{m-1}(b,c_m) \geq \Phi_{m-1}(b,c_{m-1}) \text{ for all } m \leq j.$$

Thus, we have

$$\Omega = \min\{\Phi_i(b,c) : i \in \{i', \dots, j, d\}, c \in I_i\} = \Phi_{i'}(b,c_{i'}).$$

Observe that we have two possibilities here also, that is, either $\theta_j \leq \mu$ or $\theta_j \geq \mu$. In particular,

$$\Omega = \begin{cases} \Phi_{i'}(b,c_{i'}) & \text{if } j \geq i', \\ \Phi_d(b,c^*) & \text{if } j < i'. \end{cases}$$

That is, for all i such that $\nu \leq \theta_i \leq \mu$, the bound $\Phi_i(b,c)$ is minimized at $i = i'$ with $c = c_{i'}$ if $j \geq i'$ or at $i = d$ with $c = c_*$ if $j \leq i' - 1$.

Now note that $\Phi_{i'}(b,c_{i'}) = \Phi_{i'-1}(b,c_{i'})$ and $\Phi_j(b,c^*) = \Phi_d(b,c^*)$. Thus, case 2 and case 3 yield the same bounds. That is, if $j \geq i'$, we have

$$\Omega = \Phi_{i'}(b,c_{i'}) = \Phi_{i'-1}(b,c_{i'})$$

and if $j < i'$, we have

$$\Omega = \Phi_j(b,c^*) = \Phi_d(b,c^*).$$

Now, let us investigate the two bounds arising from Cases 2 and 3.

Case A: $j \geq i'$, that is, $\theta_j \leq \mu$. Then,

$$\Omega = \Phi_{i'}(b,c_{i'-1}) = \Phi_{i'-1}(b,c_{i'-1}).$$

Note that μ is not necessarily an eigenvalue of G. But we have the bound $\Omega = \Phi_{i'}(b,c_{i'-1}) = \Phi_{i'-1}(b,c_{i'-1}) \geq \lim_{c \to \infty} \Phi(\mu,b,c) = n\frac{-\mu}{\theta_0 - \mu}$, and so $-1 \leq \mu < 0$. We have equality when $\theta_{i'} = \mu$, and hence, $n\frac{-\mu}{\theta_0-\mu}$ becomes a bound on α_3.

Case B: $j < i'$, that is, $\mu \leq \theta_j < \theta_0$. We have

$$\Omega = \Phi_d(b,c^*) = \Phi_j(b,c^*).$$

We will investigate this further.

Local minimum of $p(x)$ occurs at $x = \tau \geq \mu$. So, if

$$\lambda(p) = p(\theta_d) = p(\tau),$$

then

$$c = -(\tau^2 + \theta_d\tau + \theta_d^2) - b(\theta_d + \tau). \tag{4.2.6}$$

Substituting (4.2.6) into Equation (4.2.5), we have

$$\Phi(b) = n\frac{\triangle + b\theta_0 + (b\tau\theta_d + \tau\theta_d^2 + \tau^2\theta_d)}{(\theta_0 + b + \tau + \theta_d)(\theta_0 - \tau)(\theta_0 - \theta_d)},$$

and differentiating with respect to b gives

$$\Phi'(b) = n\frac{(\theta_0\theta_d + \theta_0)\tau + (\theta_0^2 + \theta_0\theta_d - \triangle)}{(\theta_0 + b + \tau + \theta_d)^2(\theta_0 - \tau)(\theta_0 - \theta_d)}.$$

We are interested in where $\Phi'(b) = 0$, so $\tau = -\frac{\theta_0^2 + \theta_0\theta_d - \triangle}{\theta_0(\theta_d + 1)}$.

Let θ_s be an eigenvalue such that $\lambda(p) = p(\theta_s)$. Then, θ_s is the least eigenvalue of G such that $\theta_s \geq \tau$ or the largest eigenvalue of G such that $\theta_s \leq \tau$. Hence, we want b and c that will give $\lambda(p) = p(\theta_d) = p(\theta_s)$, this being a necessary condition. So, we have

$$c = -(\theta_s^2 + \theta_d\theta_s + \theta_d^2) - b(\theta_d + \theta_s). \tag{4.2.7}$$

Substitute (4.2.7) into $p(x)$ and denote it as $p_b(x)$. We now proceed to find b.

We note that, if $\tau = \theta_s = -\frac{\theta_0^2 + \theta_0\theta_d - \triangle}{\theta_0(\theta_d + 1)}$, then $\Phi(b)$ is a constant function of b. Thus any value of b that ensures the minimum still occurs at θ_s will give us an optimal bound. That is, the domain for b must be such that, $\lambda(p_b)$ will always occur at θ_s. Now let us solve for the domain of b. We have that b satisfies $p_b(\theta_s) \leq p_b(\theta_{s-1})$ with strict inequality if $s = 1$, and $p_b(\theta_s) \leq p_b(\theta_{s+1})$.

Firstly, if we solve $p_b(\theta_s) \leq p_b(\theta_{s+1})$, that is

$$\begin{aligned}\theta_s^3 + b\theta_2 - (\theta_s^2 + \theta_d\theta_s + \theta_d^2)\theta_s - b(\theta_d + \theta_s)\theta_s \leq \;& \theta_{s+1}^3 + b\theta_2 - (\theta_s^2 + \theta_d\theta_s + \theta_d^2)\theta_{s+1} - \\ & b(\theta_d + \theta_s)\theta_{s+1},\end{aligned}$$

we get

$$\begin{aligned} b(\theta_s - \theta_{s+1})(\theta_{s+1} - \theta_d) &\leq (\theta_{s+1} - \theta_s)(\theta_{s+1} - \theta_d)(\theta_{s+1} + \theta_s + \theta_d) \\ b &\leq -(\theta_s + \theta_{s+1} + \theta_d). \end{aligned} \tag{4.2.8}$$

Secondly, if $1 < s \leq d - 1$, then solving $p_b(\theta_s) \leq p_b(\theta_{s-1})$ gives

$$b(\theta_{s-1} - \theta_s)(\theta_d - \theta_{s-1}) \leq (\theta_{s-1} - \theta_s)(\theta_{s-1} - \theta_d)(\theta_{s-1} + \theta_s + \theta_d)$$

$$b \geq -(\theta_s + \theta_{s-1} + \theta_d), \tag{4.2.9}$$

and if $s = 1$, then in order to satisfy the condition $\lambda(p_b) = p_b(\theta_1) < p_b(\theta_0)$, b must be such that $b > -(\theta_1 + \theta_0 + \theta_d)$. Hence, if τ is an eigenvalue, θ_s of G, then

$$-(\theta_s + \theta_{s-1} + \theta_d) \leq b \leq -(\theta_s + \theta_{s+1} + \theta_d), \tag{4.2.10}$$

with a strict lower inequality when $s = 1$.

On the other hand, if $\tau = -\frac{\theta_0^2 + \theta_0\theta_d - \triangle}{\theta_0(\theta_d + 1)}$ is not an eigenvalue of G, then we can choose θ_s to be either the largest eigenvalue less than τ or the least eigenvalue greater than τ.

- If we choose θ_s to be the largest eigenvalue less than τ, then $\Phi(b)$ is an increasing function with a vertical asymptote at $b = -(\theta_0 + \theta_s + \theta_d)$. We must pick the smallest b that ensures $\lambda(p_b)$ still occurs at θ_s. Thus, b must satisfy $p_b(\theta_s) = p_b(\theta_{s-1})$ yielding $b = -(\theta_1 + \theta_0 + \theta_d)$ if $1 < s \leq d - 1$, and if $s = 1$, then $b < -(\theta_1 + \theta_0 + \theta_d)$.

- On the other hand, if we choose θ_s to be the least eigenvalue greater than τ, then $\Phi(b)$ is a decreasing function with a vertical asymptote at $b = -(\theta_0 + \theta_s + \theta_d)$. We must pick the largest b that ensures $\lambda(p)$ still occurs at θ_s. Thus, b must satisfy $p_b(\theta_s) = p_b(\theta_{s+1})$ yielding $b = -(\theta_s + \theta_{s+1} + \theta_d)$.

Either of the above choices of θ_s will yield the same optimal bound since in each case $\lambda(p) = p(\theta_d) = p(\theta_s)$. Thus, we get a family of optimal polynomials. So, for simplicity, we choose θ_s to be the least eigenvalue greater or equal to τ and then take $b = -(\theta_s + \theta_{s+1} + \theta_d)$. Now substituting b into (4.2.7), we obtain $c = \theta_d\theta_s + \theta_d\theta_{s+1} + \theta_s\theta_{s+1}$. Finally, substituting $t = s$ or $t = d$ into (4.2.5), and using b and c above, we obtain the desired result in (4.2.1).

Now the quotient matrix B of $p(A)$ resulting from the proof of Theorem 3.2.3 in [2] is

$$B = \begin{bmatrix} \frac{1}{r}\sum_{u \in U}(p(A))_{uu} & p(\lambda_1) - \frac{1}{r}\sum_{u \in U}(p(A))_{uu} \\ \frac{rp(\lambda_1) - \sum_{u \in U}(p(A))_{uu}}{n-r} & p(\lambda_1) - \frac{rp(\lambda_1) - \sum_{u \in U}(p(A))_{uu}}{n-r} \end{bmatrix}, \tag{4.2.11}$$

with corresponding eigenvalues $\mu_1 \geq \mu_2$, and by interlacing

$$\lambda(p) \leq \mu_2 \leq W(p) - \frac{rp(\lambda_1) - rW(p)}{n - r}. \tag{4.2.12}$$

So, if equality holds in (4.2.1), then from (4.2.12) we conclude that $\mu_2 = \lambda(p)$ and, since $\mu_1 = p(\lambda_1)$, the interlacing is tight and the partition of $p(A)$ is regular (or equitable). Also, to derive its quotient matrix B given in (4.2.2), we use (4.2.11) with the optimal polynomial

$$p(x) = x^3 - (\theta_s + \theta_{s+1} + \theta_d)x^2 + (\theta_d\theta_s + \theta_d\theta_{s+1} + \theta_s\theta_{s+1})x$$

and the bound on $\alpha_3 = r$ in (4.2.1). Note that $W(p) = \frac{1}{r}\sum_{u\in U}(p(A))_{uu}$. Thus,

$$B_{11} = W(p) = \triangle + b\theta_0 = \triangle - (\theta_s + \theta_{s+1} + \theta_d)\delta.$$

We also have that $B_{12} = p(\delta) - W(p)$, so

$$B_{12} = \delta^3 - (\theta_s + \theta_{s+1} + \theta_d)\delta^2 + (\theta_d\theta_s + \theta_d\theta_{s+1} + \theta_s\theta_{s+1} + \theta_s + \theta_{s+1} + \theta_d)\delta - \triangle.$$

We have

$$B_{21} = \frac{r}{n-r}(p(\delta) - W(p)) = \triangle - (\theta_s + \theta_{s+1} + \theta_d)\delta - \theta_s\theta_{s+1}\theta_d.$$

Finally, $B_{22} = p(\delta) - B_{21}$ so

$$B_{22} = \delta^3 - (\theta_s + \theta_{s+1} + \theta_d)\delta^2 + (\theta_d\theta_s + \theta_d\theta_{s+1} + \theta_s\theta_{s+1} + \theta_s + \theta_{s+1} + \theta_d)\delta \\ + \theta_s\theta_{s+1}\theta_d - \triangle.$$

∎

Remark 4.2.3. A polynomial p satisfying $p(\theta_0) > \lambda(p)$ is optimal for $k = 3$ if and only if

$$\lambda(p) = p(\theta_d) = p(\theta_s) = p(\theta_{s+1}),$$

where θ_s is the least eigenvalue such that $\theta_s \geq -\frac{\theta_0^2 + \theta_0\theta_d - \triangle}{\theta_0(\theta_d + 1)}$.

Observe that, if G has girth greater than 3, then $\triangle = 0$, and the bound in Theorem 4.2.2 becomes as follows.

Corollary 4.2.4. Let G be a δ-regular graph with n vertices, with girth greater than 3, and distinct adjacency eigenvalues $\delta = \theta_0 > \theta_1 > \cdots > \theta_d$, with $d \geq 3$. Let θ_s be the least eigenvalue such that $\theta_s \geq -\frac{\theta_d + \theta_0}{\theta_d + 1}$. Then,

$$\alpha_3 \leq n\frac{-\theta_0(\theta_s + \theta_{s+1} + \theta_d) - \theta_s\theta_{s+1}\theta_d}{(\theta_0 - \theta_s)(\theta_0 - \theta_{s+1})(\theta_0 - \theta_d)}. \qquad (4.2.13)$$

The subsequent chapter delves into exploring various applications stemming from Theorem 4.2.2.

Chapter 5

Hamming and Johnson Graphs and other Applications of the 3-Independence Bound

In this chapter, we explore applications arising from Theorem 4.2.2, determining 3-independence bounds for well-known graph families. Additionally, we construct some 3-independent sets for specific Hamming graphs.

5.1 Diameter of a Graph

As a collateral benefit of Theorem 3.2.1, one can derive upper bounds for the diameter of a graph G. This stems from the observation that if $\alpha_k = 1$, the graph's diameter is at most k. To establish $\alpha_k = 1$, it suffices to secure an upper bound less than 2. The following result is thus an immediate consequence of Theorem 4.2.2.

Corollary 5.1.1. Let G be a δ-regular graph with n vertices, adjacency matrix A, and distinct eigenvalues $\delta = \theta_0 > \theta_1 > \cdots > \theta_s > \theta_{s+1} > \ldots, > \theta_d$, with $d \geq 3$. Let θ_s be the least eigenvalue such that $\theta_s \geq -\frac{\theta_0^2+\theta_0\theta_d-\triangle}{\theta_0(\theta_d+1)}$, where $\triangle = \max_{u\in V}\{(A^3)_{uu}\}$, twice the largest number of triangles on any vertex in G. If

$$n\frac{\triangle - \theta_0(\theta_s + \theta_{s+1} + \theta_d) - \theta_s\theta_{s+1}\theta_d}{(\theta_0 - \theta_s)(\theta_0 - \theta_{s+1})(\theta_0 - \theta_d)} < 2, \tag{5.1.1}$$

then G has diameter at most 3.

5.2 Antipodal Bipartite Distance-Regular Graphs

We consider an infinite family of graphs where the bound in Theorem 4.2.2 is tight.

Definition 5.2.1. Let G be a connected graph. For a vertex $u \in V(G)$, we define $V_i(u)$ to be the set of vertices at distance i from u. Then, G is a *distance-regular graph* if $|V_i(u) \cap V_j(v)|$ depends only on the distance between vertices u and v.

Thus, given any two vertices u and v at distance k in a distance-regular graph G, the number of vertices at distance i from u and distance j from v is determined by k, i, j. An *intersection array* of a distance regular graph G of diameter d is a sequence of integers $\{b_0, b_1, \ldots, b_{d-1}; c_1, \ldots, c_d\}$ such that for all $1 \leq k \leq d$, b_k is the number of neighbours of u at distance $k+1$ from v and c_k is the number of neighbours of u at distance $k-1$ from v. For a detailed treatment of distance-regular graphs, see Brouwer, Cohen and Neumaier [12].

A graph G of diameter d is *antipodal* if there exists a partition of the vertex set into classes with the property that any two distinct vertices in the same class are at distance d, while two vertices in different classes are at distance less than d.

Let G be an antipodal bipartite distance-regular graph, with degree δ and diameter 3. These graphs have $n = 2(\delta + 1)$ vertices (Brouwer, Cohen and Neumaier [12]), intersection array $\{\delta, \delta - 1, 1; 1, \delta - 1, \delta\}$, and distinct eigenvalues

$$\theta_0 = \delta,\ \theta_1 = 1,\ \theta_2 = -1,\ \theta_3 = -\delta. \tag{5.2.1}$$

As G is bipartite, $\theta_s = 1$. Thus, by Theorem 4.2.2, we have

$$\begin{aligned} \alpha_3 &\leq 2(\delta + 1)\frac{\delta - (1-1) + (1)(-1)}{2(\delta - 1)(\delta + 1)} \\ &= 2(\delta + 1)\frac{(\delta - 1)}{2(\delta - 1)(\delta + 1)} = 1 \end{aligned}$$

as expected since G has diameter 3. Also, since $b = \delta$ and $c = -1$, the polynomial that gives this bound is $p(x) = x^3 + \delta x^2 - x$.

If the adjacency matrix of the graph is $\mathbf{A}$, then we have that the matrix $p(\mathbf{A}) = \mathbf{A}^3 + \delta \mathbf{A}^2 - \mathbf{A}$ has a regular partition with the quotient matrix

$$B = \begin{bmatrix} \delta^2 & 2\delta^3 - \delta^2 - \delta \\ \delta^2 + \delta & 2\delta^3 - \delta^2 - 2\delta \end{bmatrix}.$$

5.3 Hamming Graphs

Let $d \geq 3$ and $q \geq 2$ be integers, and let Q be a set of q elements. The Hamming graph $H(d, q)$ is a $d(q-1)$-regular graph with vertex set Q^d, consisting of sequences of length d from Q and two sequences (vertices) are adjacent if they differ in just one position. A 3-independent set in $H(d, q)$ thus, consists of sequences that pairwise differ in at least 4 positions. $H(d,q)$ has q^d vertices and eigenvalues $d(q-1)-qi$ for $i=0,1,\dots,d$ with respective multiplicities $\binom{d}{i}(q-1)^i$. See Brouwer and Haemers [14]. Also, $\triangle = 2d\binom{q-1}{2} = d(q-1)(q-2)$, $\theta_0 = d(q-1)$, $\theta_d = -d$ and s is the largest index such that

$$\begin{aligned}\theta_s &\geq -\frac{\theta_0^2+\theta_0\theta_d-\triangle}{\theta_0(\theta_d+1)}\\ &= -\frac{d^2(q-1)^2-d(q-1)d-d(q-1)(q-2)}{d(q-1)(-d+1)}\\ &= -\frac{d(q-1)-d-(q-2)}{(-d+1)} = \frac{(d-1)(q-2)}{d-1} = q-2.\end{aligned}$$

Thus, s is the largest index such that $\theta_s \geq q-2$. Solving $\max\{s : d(q-1)-sq \geq q-2\}$, that is,

$$\begin{aligned}d(q-1)-sq &\geq q-2\\ d-1-\frac{d-2}{q} &\geq s\\ d-1-\left\lceil\frac{d-2}{q}\right\rceil &= s.\end{aligned}$$

Let $b = d \mod q$. (Note that b in this chapter has no relation with b in the optimal polynomial). Now, $d = aq+b$ for some $a \in \mathbb{Z}$, so

$$\begin{aligned}s &= d-1-\left\lceil\frac{d-2}{q}\right\rceil\\ &= d-1-\left\lceil\frac{aq+b-2}{q}\right\rceil\\ &= d-1-a-\left\lceil\frac{b-2}{q}\right\rceil.\end{aligned}$$

Now if $q=2$, we have

$$s = d-1-a-\left\lceil\frac{b-2}{q}\right\rceil = d-a-\left\lceil\frac{b}{2}\right\rceil = \begin{cases} d-a \text{ if } b=0\\ d-a-1 \text{ if } b=1.\end{cases}$$

Similarly, if $q>2$, we have

$$s = d-1-a-\left\lceil\frac{b-2}{q}\right\rceil = \begin{cases} d-a-1 \text{ if } 0\leq b\leq 2\\ d-a-2 \text{ if } 2<b<q.\end{cases}$$

Now, substituting the index s, we have $\theta_s = 0$ and $\theta_{s+1} = -2$ if $q=2$ and $b=0$, otherwise

$$\theta_s = \begin{cases} -b+q \text{ if } 0\leq b\leq 2\\ -b+2q \text{ if } 2<b<q,\end{cases}$$

and

$$\theta_{s+1} = \begin{cases} -b \text{ if } 0 \leq b \leq 2 \\ -b+q \text{ if } 2 < b < q. \end{cases}$$

We deduce the following from Theorem 4.2.2.

Proposition 5.3.1. Let $b = d \mod q$. The 3-independence number of the Hamming graph $H(d,q)$ satisfies the following.

$$\alpha_3(H(d,q)) \leq \begin{cases} q^{d-1}\dfrac{d-2}{d(d(q-1)-q)} \text{ if } b=0 & (5.3.1) \\ q^{d-1}\dfrac{1}{d(q-1)+1} \text{ if } b=1 & (5.3.2) \\ q^{d-1}\dfrac{1}{d(q-1)-q+2} \text{ if } b=2 & (5.3.3) \\ q^{d-1}\dfrac{q(d-b)+(b-1)^2+(1-d)}{(dq-d+b-2q)(dq-d+b-q)} \text{ if } 2<b<q. & (5.3.4) \end{cases}$$

It is easy to see that for $d = q$, the bound on $H(d,q)$ is an integer. Indeed, $\alpha_3(H(d,d)) = \alpha_3(H(q,q)) \leq q^{q-3} \in \mathbb{Z}^+$. More generally, we have an integer bound on $H(d,q)$ for $3 \leq d \leq q+2$ with $q \geq 2$. Observe that $b = d$ for $d \in [3, q-1]$, so substituting $b = d$ into Equation (5.3.4) of Proposition 5.3.1, we have an integer bound q^{d-3}. Moreover, we have $b = 0$, $b = 1$ and $b = 2$ for $H(q,q)$, $H(q+1,q)$ and $H(q+2,q)$ respectively, hence, Equations (5.3.1-5.3.3) each yields an integer bound q^{d-3} for each case. We summarize this result below.

Corollary 5.3.2. Given $3 \leq d \leq q+2$, the right side of Equations (5.3.1-5.3.4) simplifies to q^{d-3}, therefore

$$\alpha_3(H(d,q)) \leq q^{d-3}. \qquad (5.3.5)$$

The Singleton bound [66] (on the number of codewords in a code of length d and minimum distance 4) gives $\alpha_3 \leq q^{d-3}$ for all d and q, and when $d > q+2$ the ratios of the right sides of the bounds in Proposition 5.3.1 to the Singleton bound approach 0 as d approaches infinity.

Now, when $b = 1$, bound (5.3.2) is an integer if $d = \frac{q^r-1}{q-1}$ with $r \in \mathbb{Z}^+$. To see this, observe that the denominator of the bound is

$$d(q-1)+1 = \frac{q^r-1}{q-1}(q-1)+1 = q^r.$$

Thus,

$$\alpha_3(H(d,q)) \leq \frac{q^{d-1}}{d(q-1)+1} = \frac{q^{\frac{q^r-1}{q-1}-1}}{q^r} = q^{\frac{q^r-q}{q-1}-r} \in \mathbb{Z}^+.$$

Similarly, when $b = 2$, bound (5.3.3) is an integer if $d = \frac{q^r+(q-2)}{q-1}$ with $r \in \mathbb{Z}^+$. Observe that the denominator of the bound is

$$d(q-1) - q + 2 = \frac{q^r + (q-2)}{q-1}(q-1) - q + 2 = q^r.$$

Thus,

$$\alpha_3(H(d,q)) \leq \frac{q^{d-1}}{d(q-1)-q+2} = \frac{q^{\frac{q^r-1}{q-1}}}{q^r} = q^{\frac{q^r-1}{q-1}-r} \in \mathbb{Z}^+.$$

Hence, one can study tightness at these values of d and q that lead to integer bounds. Let us now consider some special Hamming graphs and investigate their tightness.

5.3.1 The Hamming Graph $H(3,q)$

Consider the Hamming graph $H(3,q)$. It has q^3 vertices and the distinct eigenvalues $3q-3, 2q-3$, $q-3$ and -3. Bang, van Dam and Koolen [6] showed $H(3,q)$ is uniquely determined by its spectrum for $q \geq 36$. Now, $3 \mod q$ is $0, 1$ or 2 for $q \geq 2$. Thus, the upper bound of Equation (5.3.2) is exactly 1 for $\alpha_3(H(3,q))$, as expected, since $H(3,q)$ has diameter 3.

5.3.2 The Hamming Graph $H(4,q)$

Considering the Hamming graph $H(4,q)$, Corollary 5.3.2 implies $\alpha_3(H(4,q)) \leq q$, and this bound is tight. An illustrative 3-independent set is $\{1111, 2222, 3333, \ldots, qqqq\}$, showcasing its cardinality of q.

5.3.3 The Hamming Graph $H(5,q)$

Corollary 5.3.2 establishes $\alpha_3(H(5,q)) \leq q^2$. We now proceed to investigate its tightness. Recall a *Latin square* L of order q is an $q \times q$ array in which q distinct symbols $\{1, 2, 3, \ldots, q\}$ are arranged so that each symbol occurs exactly once in each row and column. Two Latin squares L_1 and L_2 of order q are said to be *orthogonal* if when superimposed, each of the possible q^2 pairs occurs exactly once. A set of Latin squares is said to be *mutually orthogonal* if the Latin squares are pairwise orthogonal. This set is termed Mutually Orthogonal Latin Square (MOLS). Suppose ℓ is the number of MOLS of size q that exists, then since each Latin square is a

$q \times q$ matrix, we can create q^2 words of length $\ell + 2$ by creating an orthogonal array (OA) of q^2 rows and $\ell + 2$ columns from the MOLS (see Stinson [66]). We now show the rows of this array form a code with minimum distance $\ell + 1$. Suppose the ℓ MOLS $L_1, L_2, \ldots, L_\ell$ are defined on the q elements set $\{1, 2, \ldots, q\}$, and has rows and columns labelled by $\{1, 2, \ldots, q\}$. For every $i, j \in \{1, 2, \ldots, q\}$, construct the $(2 + \ell)$-tuple $(i, j, L_1(i, j), L_2(i, j), \ldots, L_\ell(i, j))$, where $L_l(i, j)$ refers to the element in the ith row and jth column of the Latin square L_l. The orthogonal array from this MOLS is a $q^2 \times (2 + \ell)$ array where the rows consist of the $(2 + \ell)$-tuples $(i, j, L_1(i, j), L_2(i, j), \ldots, L_\ell(i, j))$. To see that these q^2 codes (rows of the OA) are $\ell + 1$-independent, consider a pair ρ_u and ρ_v of rows of the orthogonal array. Let $\rho_u = (i, j, L_1(i, j), L_2(i, j), \ldots, L_\ell(i, j))$ and $\rho_v = (k, l, L_1(k, l), L_2(k, l), \ldots, L_\ell(k, l))$. We consider 3 cases.

A. If $i = k$. In this case, we have same rows of MOLS, so $j \neq l$ (by the construction of the OA, j and l represent the column numbers of the Latin squares). Moreover, $L_{i^*}(i, j) \neq L_{i^*}(k, l)$ for all $1 \leq i^* \leq \ell$ since $L_{i^*}(i, j)$ and $L_{i^*}(k, l)$ are elements on the row of a Latin square and hence, distinct. Thus, if $i = k$, the Hamming distance $d(\rho_u, \rho_v) = \ell + 1$.

B. If $j = l$. That is, we have the same column numbers of the Latin squares, thus, the rows i and k are different and $L_{i^*}(i, j) \neq L_{i^*}(k, j)$. Thus, the Hamming distance $d(\rho_u, \rho_v) = \ell + 1$.

C. If $L_{i^*}(i, j) = L_{i^*}(k, j)$ for any $1 \leq i^* \leq \ell$. Note $L_{i^*}(i, j)$ and $L_{i^*}(k, j)$ come from the same Latin square L_{i^*} and thus, must be from different row and column of L_{i^*}. That is, $i \neq k$ and $j \neq l$. Moreover, for $i^* \neq j^*$, $L_{j^*}(i, j) \neq L_{j^*}(k, j)$ since the two Latin squares L_{i^*} and L_{j^*} are orthogonal. Otherwise, when L_{i^*} and L_{j^*} are superimposed, we will have the pair $(L_{i^*}(i, j), L_{j^*}(i, j))$ twice, contradicting MOLS. Thus, the Hamming distance $d(\rho_u, \rho_v) = \ell + 1$.

In each case, the Hamming distance is $\ell + 1$. Thus, MOLS codes give constructions for a 3-independent set of $H(5, q)$ that meet our bound when there are at least $\ell = 3$ MOLS of size q. For instance, for q a prime power, $l = q - 1$. From Hanani [45], Wilson [67] and the survey work of Colbourn and Dinitz [21], we know the lower bounds on ℓ for $q \geq 3$. Thus, since $\ell \geq 3$ for $q \geq 3$ except for $q = 3, 6$ and possibly for $q = 10$, we have a 3-independent set for $H(5, q)$ which meets our bound.

5.3.4 The Hamming Graph $H(d, 3)$

The Hamming graph $H(d, 3)$ has distinct eigenvalues $2d - 3i$ for $i = 0, 1, 2, \ldots, d$. It has $\triangle = 2d$, $\theta_s = 3 - b$ and $\theta_{s+1} = -b$, where $b = d \mod 3$. We have the following bound for $H(d, 3)$.

Corollary 5.3.3. Let $b = d \mod 3$. The 3-independence number of the Hamming graph $H(d, 3)$ satisfies the following.

$$\alpha_3(H(d,3)) \leq 3^{d-1}\frac{2d + b^2 + b - 4}{(2d + b)(2d + b - 3)}. \tag{5.3.6}$$

Alternatively,

$$\alpha_3(H(d,3)) \leq \begin{cases} 3^{d-1}\frac{d-2}{d(2d-3)} \text{ if } b = 0 \\ \\ \frac{3^{d-1}}{2d+1} \text{ if } b = 1 \\ \\ \frac{3^{d-1}}{2d-1} \text{ if } b = 2. \end{cases} \tag{5.3.7}$$

It is easily verified that the bound in (5.3.7) is tight for $d = 3$. Note that the bound is an integer when $d = \frac{3^r-1}{2}$ for $b = 1$, and when $d = \frac{3^r+1}{2}$ for $b = 2$ for all $r \in \mathbb{Z}^+$. It is also an integer when $d = 6$. Using GAP, we confirm $H(6, 3) = 18$, meaning it is tight. It's however not tight for $H(5, 3)$, as the bound is 9 but actual value is 6. Thus, the bound (5.3.7) is not tight in general.

5.3.5 The Hamming Graph $H(d, 2)$

Consider the Hamming graph $H(d, 2)$ also known as the hypercube Q_d or the d-cube. The vertices of this graph are binary sequences (hence forth, sequences) of length d and two sequences (vertices) are adjacent if they differ in just one position. Thus, it has 2^d vertices. Suppose the matrix $\mathbf{A}$ is its adjacency matrix. Then, its eigenvalues are the integers $d - 2i$, for $i = 0, ..., d$ with respective multiplicities $\binom{d}{i}$. See Brouwer and Haemers [14] for further details. It is bipartite and so $\triangle = 0$ and $\theta_0 = -\theta_d = d$. If its diameter d is odd, then $\theta_s = 1$ and $\theta_{s+1} = -1$. Moreover, if d is even, then $\theta_s = 0$ and $\theta_{s+1} = -2$. Thus, by Theorem 4.2.2, we have the following.

Corollary 5.3.4. The 3-independence number of the Hamming graph $H(d, 2)$ satisfies the following.

$$\alpha_3(H(d,2)) \leq \begin{cases} 2^d\dfrac{d-(1-1)-1}{2(d-1)(d+1)} = \dfrac{2^{d-1}}{d+1} \text{ if } d \text{ is odd} & (5.3.8) \\ \\ 2^d\dfrac{d-(0-2)}{2(d)(d+2)} = \dfrac{2^{d-1}}{d} \text{ if } d \text{ is even.} & (5.3.9) \end{cases}$$

This bound coincides with the bound of Fiol in [31].

In what follows, we construct a 3-independent set and thus, a lower bound for $\alpha_3(H(d, 2))$. We then show that bound (5.3.9) is tight for some family of d, specifically $d = 2^r$, while bound (5.3.8) is tight for $d = 2^r - 1$, for all $r \in \mathbb{Z}^+$.

5.3.6 A 3-independent Set for $H(d, 2)$

We first present a general result, which we prove by presenting a construction of a 3-independent set.

Theorem 5.3.5. *Let $d_1 \leq d_2$. Suppose the Hamming graphs $H(d_1, 2)$ and $H(d_2, 2)$ have 3-independent sets of size ℓ_1 and ℓ_2 respectively. Then $\alpha_3(H(d_1+d_2, 2)) \geq \ell_1\ell_2 d_1$.*

Proof: Given $d_1 \leq d_2$, take a 3-independent set U of size ℓ_1 in $H(d_1, 2)$ and a 3-independent set V of size ℓ_2 in $H(d_2, 2)$. We construct a 3-independent set of size $\ell_1\ell_2 d_1$ in $H(d_1 + d_2, 2)$. Let $W = U \times V$ be the cartesian product of U and V. Thus, the size of W is $\ell_1\ell_2$. Any pair of sequences x_1y_1 and x_2y_2 in W with $x_1, x_2 \in U$ and $y_1, y_2 \in V$, are such that $x_1 \neq x_2$ or $y_1 \neq y_2$ or both. So, x_1y_1 and x_2y_2 are 3-independent in W since x_1 and x_2 are 3-independent in U or y_1 and y_2 are 3-independent in V. Hence, W is a 3-independent set. For each $j = 1, 2, .., d_1$, let W_j be the set of sequences resulting from adding $1 \mod 2$ to the j and (d_1+j)th elements of each sequence in W. (Hence forth, we shall say the ith column of a sequence is flipped when $1 \mod 2$ is added to the ith element of the sequence). This results in a set $A = \bigcup_{j=1}^{d_1} W_j$ of size $\ell_1\ell_2 d_1$. We claim set A is 3-independent. For simplicity, assume the sequences in a set are rows of a matrix representing the set. First of all, any pair of sequences from the same $W_j \in A$ is a result of flipping the same columns of sequences in W, so their Hamming distance remains unchanged. Also, any pair of sequences each from W_i and W_j, with $i \neq j$, either resulted from the same sequence or two distinct sequences of W. If the pair are from the same sequence, then we have 4 distinct columns of the sequence flipped, two for each pair. Hence, the pair of sequences have a Hamming distance exactly 4. On the other hand, if the pair is from two distinct sequences, then at least four out of their Hamming distance came from either the first d_1 columns or the last d_2 columns, so the flip reduced the Hamming distance by at most two in that half but also gained two in the other half. Hence, the Hamming distance remains at least 4. Thus, we have obtained a 3-independent set A for $H(d_1 + d_2, 2)$ of size $\ell_1\ell_2 d_1$ proving the claim. ∎

An immediate consequence of Theorem 5.3.5 is as follows. If $d = d_1 = d_2$ and $\alpha_3(H(d, 2)) = \ell$, then we have obtained a 3-independent set A for $H(2d, 2)$ of size $d\ell^2$. We now show by induction that it coincides with the upper bound (5.3.9) when $d = 2^r$, for all $r \in \mathbb{Z}^+$, and thus, tight. It is clear that for $r = 1$, that is, $d = 2$, we have just one element in the 3-independent set, say 00. Suppose we have a 3-independent set in $H(d, 2)$ of size $\ell = \dfrac{2^{d-1}}{d}$ for $d = 2^r$, then the construction gives $d\ell^2 = \dfrac{2^{2d-1}}{2d}$ for $2^{r+1} = 2d$. But $\dfrac{2^{2d-1}}{2d} = \alpha_3(H(2d, 2))$, using bound (5.3.9). We have thus, shown that the bound (5.3.9) is tight when $d = 2^r$, and also proved the following result.

Corollary 5.3.6. If $\alpha_3(H(d,2)) = \ell$, then $\alpha_3(H(2d,2)) \geq d\ell^2$ with equality if $d = 2^r$, for all $r \in \mathbb{Z}^+$.

In the case where equality is attained, Theorem 4.2.2 tells us more. We have the following.

Corollary 5.3.7. Let $\mathbf{A}$ be the adjacency matrix of the Hamming graph $H(d,2)$ with $d = 2^r$, for all $r \in \mathbb{Z}^+$. Then, the matrix $\mathbf{A}^3 + (2+d)\mathbf{A}^2 + 2d\mathbf{A}$ has a regular partition (with a set of $\frac{2^{d-1}}{d}$ 3-independent vertices and their complement) with the quotient matrix

$$\mathbf{B} = \begin{bmatrix} d^2+2d & d^3+2d^2 \\ d^2+2d & 2d^3+3d^2-2d \end{bmatrix}.$$

Recall the elements of the quotient matrix $\mathbf{B}$ are obtained from

$$\begin{aligned} B_{11} &= 0 - (-2-d)d = d^2+2d \\ B_{12} &= d^3 - (-2-d)d + (2d-2-d) - 0 = d^3+2d \\ B_{21} &= 0 - (-2-d)d - 0 = d^2+2d \\ B_{22} &= d^3 - (-2-d)d + (2d-2-d)d + 0 - 0 = 3d^2-2d. \end{aligned}$$

Let X be a set of cardinality n, consisting of sequences of length d. Create a matrix $\mathbf{X}_{n,b}$ from X by making each of the n sequences a row. We say X is *balanced* if each column of $\mathbf{X}_{n,b}$ has as many 1s as 0s. We show briefly that the constructed 3-independent set A in the proof of Theorem 5.3.5 above is balanced for all $r > 1$. Suppose we start with a balanced 3-independent set W. Note that for $r = 2$, the construction gives a 3-independent set as $W = \{1010, 0101\}$ which is balanced. Now, W^2 is also balanced since it is a concatenation of sequences of a balanced set. Moreover, W_j^2 is balanced since flipping the j and $j+d$ columns of sequences of W^2 just swaps 0s and 1s in those columns. Thus, A is balanced, being the union of balanced sets.

Now, as corollary of the construction above, we can construct 3-independent sets and thus, lower bounds of $\alpha_3(H(l,2))$ for $\frac{1}{2}d < l < d$. We start with a 3-independent set in $H(d,2)$ of size ℓ with $d = 2^r$. Recall that this set is balanced for all $r \geq 2$. Pick any column and take the sequences that contain a 1 in that column. Delete these 1s and we have found a set of sequences of length $d-1$. It is easy to see that this set is still 3-independent, and thus, a 3-independent set of size $\frac{1}{2}\ell$ in $H(d-1,2)$. We summarize the above in the following.

Proposition 5.3.8. The 3-independence number of the Hamming graph satisfies

$$\alpha_3(H(d-1,2)) \geq \frac{1}{2}\alpha_3(H(d,2)).$$

Thus, recursively, we can construct a 3-independent set for $H(l,2)$ for all $\frac{1}{2}d < l < d$ where $d = 2^r$, for all $r \in \mathbb{Z}^+$

Proposition 5.3.9. The 3-independence number of the Hamming graph satisfies

$$\alpha_3(H(d-i,2)) \geq \frac{2^{d-(i+1)}}{d} \tag{5.3.10}$$

with $0 \leq i \leq \frac{1}{2}(d-2)$ and $d = 2^r$, for all $r \in \mathbb{Z}^+$.

An immediate consequence of this is that bound (5.3.8) is tight for $d = 2^r - 1$ for all $r \in \mathbb{Z}^+$. To see this, we know that for $d = 2^r$ we have

$$\alpha_3(H(d,2)) = \frac{2^{d-1}}{d}.$$

So, from Proposition 5.3.8, we have

$$\alpha_3(H(d-1,2)) \geq \frac{1}{2}\alpha_3(H(d,2)) = \frac{1}{2}\frac{2^{d-1}}{d} = \frac{2^{d-2}}{d},$$

while from bound (5.3.8), we have

$$\alpha_3(H(d-1,2)) \leq \frac{2^{(d-1)-1}}{(d-1)+1} = \frac{2^{d-2}}{d}.$$

Thus,

$$\alpha_3(H(d-1,2)) = \frac{2^{d-2}}{d},$$

proving that bound (5.3.8) is tight for $d-1 = 2^r - 1$ for all $r \in \mathbb{Z}^+$. That is,

$$\alpha_3(H(d,2)) = \frac{2^{d-1}}{d}$$

for $d = 2^r - 1$ for all $r \in \mathbb{Z}^+$.

The following is immediate.

Corollary 5.3.10. Let $\mathbf{A}$ be the adjacency matrix of the Hamming graph $H(d,2)$ with $d = 2^r - 1$, for all $r \in \mathbb{Z}^+$. Then, the matrix $\mathbf{A}^3 + d\mathbf{A}^2 - \mathbf{A}$ has a regular partition (with a set of $\frac{2^{d-1}}{d+1}$ 3-independent vertices and their complement) with the quotient matrix

$$\mathbf{B} = \begin{bmatrix} d^2 & 2d^3 - d^2 - d \\ d^2 - d & 2d^3 - d^2 - 2d \end{bmatrix}.$$

Table 5.1: Bound for some Hamming graphs $H(d,2)$

d-cube	Corollary 5.3.4	Proposition 5.3.9	α_3
2	1	1	1
3	1	1	1
4	2	2	2
5	2.6	2	2
6	5.3	4	4
7	8	8	8
8	16	16	16
9	25.6	16	20

Recall the elements of the quotient matrix $\mathbf{A}$ are

$$\begin{aligned}
B_{11} &= 0-(1-1-d)d = d^2 \\
B_{12} &= d^3-(-d)d+(-d+d-1-d)d-0 = d^3+2d \\
B_{21} &= 0-(-2-d)d-0 = d^2+2d \\
B_{22} &= d^3-(-2-d)d+(2d-2-d)d+0-0 = 3d^2-2d.
\end{aligned}$$

Observe from Table 5.1 that bound (5.3.10) in Proposition 5.3.9 is tight for all $d \leq 8$. Observe also that $\alpha_3(H(8,2)) = 16$ and $\alpha_3(H(9,2)) = 20$, so by Theorem 5.3.5 $\alpha_3(H(17,2)) \geq 2560$, while Proposition 5.3.9 gives $\alpha_3(H(17,2)) \geq \frac{2^{16}}{32} = 2048$. Hence, Theorem 5.3.5 can be stronger than Proposition 5.3.9. We can also compare the upper bounds (5.3.8 and 5.3.9) with the size of the 3-independent sets A constructed. Observe that the upper bounds (5.3.8 and 5.3.9) can be summarized as in the following proposition.

Proposition 5.3.11. The 3-independence number of the Hamming graph satisfies

$$\alpha_3(H(d-i,2)) \leq \frac{2^{d-(i+1)}}{d-i} \tag{5.3.11}$$

with $0 \leq i \leq \frac{1}{2}(d-2)$ and $d = 2^r$, for all $r \in \mathbb{Z}^+$.

Now, the ratio of the bound (taking the right side of Equation (5.3.11)) to the size of the constructed 3-independent set (taking the right side of Equation (5.3.10)) is

$$\frac{d}{d-2j}$$

for both $H(d-2j-1,2)$ and $H(d-2j,2)$ with $d = 2^r$, and $0 \leq j \leq \frac{1}{4}(d-2)$. For r fixed and $0 \leq j \leq \frac{1}{4}(d-2)$, the ratio decreases as d increases. Moreover, for $j = \frac{1}{4}(d-2)$ and r increasing, the ratio asymptotically approaches 2.

5.4 Odd Graphs

Consider also the Odd graph O_ℓ. The vertices of O_ℓ correspond to the $(\ell-1)$-element subsets of a $(2\ell-1)$-element set, and two vertices are adjacent if and only if the corresponding subsets are disjoint. The Odd graph O_ℓ is an ℓ-regular graph of order $n = \binom{2\ell-1}{\ell-1} = \frac{1}{2}\binom{2\ell}{\ell}$, diameter $D = \ell - 1$, with the integer eigenvalues $\theta_i = (-1)^i(\ell - i)$ with corresponding multiplicities $m(\theta_i) = \binom{2\ell-1}{i} - \binom{2\ell-1}{i-1}$ for $i = 0, 1, \ldots, \ell-1$. We note that O_2 is a triangle while O_3 is the Petersen graph. The girth of O_ℓ is 3 if $\ell = 2$, 5 if $\ell = 3$ and 6 if $\ell > 3$. See, for instance, Biggs [9] and Godsil [35] for more details. Observe that, for ℓ odd, the distinct eigenvalues of O_ℓ are

$$\mathrm{ev}(O_\ell) = \{\ell, -(\ell-1), (\ell-2), \ldots, 3, -2, 1\} = \{\ell, \ell-2, \ldots, 3, 1, -2, \ldots, 1-\ell\},$$

while for ℓ even, the distinct eigenvalues of O_ℓ are

$$\mathrm{ev}(O_\ell) = \{\ell, -(\ell-1), (\ell-2), \ldots, -3, 2, -1\} = \{\ell, \ell-2, \ldots, 2, -1, -3, \ldots, 1-\ell\}.$$

For $\ell > 2$, we have that $\triangle = 0$. Hence, for odd $\ell > 2$, we have $\theta_s = 1$, and $\theta_{s+1} = -2$. Similarly, for even $\ell > 2$, we have $\theta_s = 2$, and $\theta_{s+1} = -1$. Thus, by Theorem 4.2.2, we have the following.

Corollary 5.4.1. The 3-independence number of the Odd graph O_ℓ satisfies the following.

$$\alpha_3(O_\ell) \leq \frac{1}{2(2\ell-1)}\binom{2\ell}{\ell} \times \begin{cases} \dfrac{\ell^2 - 2\ell + 2}{(\ell+2)(\ell-1)} & \text{if } \ell \text{ is odd} \qquad (5.4.1) \\[2ex] \dfrac{\ell^2 - 4\ell + 2}{(\ell+1)(\ell-2)} & \text{if } \ell \text{ is even.} \qquad (5.4.2) \end{cases}$$

5.5 Johnson Graphs

Recall that the Johnson graph $J(n,k)$ has as vertices the k-element subsets of an n-element set, where two vertices are adjacent whenever the corresponding subsets intersect in exactly $k-1$ elements. It has diameter $d = \min\{k, n-k\}$ and eigenvalues $\theta_j = (k-j)(n-k-j) - j$ for $0 \leq j \leq d$ (Brouwer, Cohen and Neumaier [12]). So, we have $\theta_0 = k(k-k)$, and $\theta_d = -k$ if $d = k$ and $\theta_d = k - n$ if $d = n - k$.

We show that each vertex v in $J(n,k)$ is part of $\frac{1}{2}k(n-k)(n-2)$ triangles. Assume, without loss of generality, that $v = \{1, 2, \ldots, k\}$, and thus, v has $k(n-k)$ neighbors. Consider a neighboring vertex $w = \{2, 3, \ldots, k+1\}$. The common neighbors of v and w can either include all elements of $v \cap w = \{2, 3, \ldots, k\}$, resulting in $n-k-1$ choices for a k-th element (excluding 1 and $k+1$), or omit one element from $v \cap w$. In the latter case, the neighbor of v and w missing one element of $v \cap w$

must include both 1 and $k+1$, leading to $k-1$ ways to choose the missing element. Altogether, this yields $n-2$ common neighbors.
While this produces $k(n-k)(n-2)$ triangles containing v, we must correct for double-counting since either of the other vertices of the triangle could be the chosen neighbor w. Thus, v contributes to $\frac{1}{2}k(n-k)(n-2)$ unique triangles in $J(n,k)$.

Now, since each vertex v of $J(n,k)$ is contained in $\frac{1}{2}k(n-k)(n-2)$ triangles, we have $\triangle = k(n-k)(n-2)$. Thus, θ_s is the least eigenvalue such that

$$\theta_s \geq \frac{k(n-k)-(n+d)+2}{d-1}.$$

We can find the exact value of s, it is the floor of the smallest root of the quadratic equation $(k-j)(n-k-j)-j = \frac{k(n-k)-(n+d)+2}{d-1}$ in j. In particular, for $J(2k,k)$, that is, if $n=2k$, then θ_s is the least eigenvalue such that $\theta_s \geq k-2$ and the index s is $s = \lfloor \frac{2k+1-\sqrt{8k-7}}{2} \rfloor$. Hence, by Theorem 4.2.2, we have the following.

Corollary 5.5.1. The 3-independence number of the Johnson graph $J(2k,k)$ satisfies the following.

$$\alpha_3(J(2k,k)) \leq \frac{1}{k+1}\binom{2k}{k}\frac{\theta_s\theta_{s+1}-(\theta_s+\theta_{s+1}+2-3k)}{(k^2-\theta_s)(k^2-\theta_{s+1})}, \tag{5.5.1}$$

where $s = \lfloor \frac{2k+1-\sqrt{8k-7}}{2} \rfloor$ and $\theta_s = (k-s)^2 - s$.

In Table 5.2, we show the bounds of the 3-independence numbers for the Johnson graph $J(2k,k)$ for $k = 2, 3, \ldots, 7$ using Corollary 5.5.1.

Table 5.2: Bound for some Johnson graphs

Johnson Graph $J(2k,k)$	θ_s	θ_{s+1}	Theorem 4.2.2	α_3
J(4,2)	0	-2	1	1
J(6,3)	3	-1	1	1
J(8,4)	2	-1	2	2
J(10,5)	7	1	3.11	2
J(12,6)	6	0	7.33	4
J(14,7)	5	-1	19.5	8

5.6 Comparison of Bounds for Some Named Graphs

In Table 5.3, we compare our bounds with the bounds in Abiad, Coutinho, Fiol [2] and Fiol [31], and the actual 3-independence number (when known) for some named graphs.

Table 5.3: Comparison between different upper bounds for the 3-independence number of some graphs.

Graph	Bound in (3.2.6) [2]	Bound in (3.2.9) [31]	Theorem 4.2.2	α_3
Johnson Graph J(14,7)	26.74	19.5	19.5	8
Cube Graph(8)	114.25	16	16	16
Odd Graph(6)	141.27	21	21	15
Balaban 10-cage	28	12.82	11.67	9
Frucht graph	3.62	2.35	2.25	2
Meredith graph	27.48	9.18	8.58	7
Moebius-Kantor graph	6.4	2	2	2
Bidiakis cube	3.66	1.92	1.50	1
Gosset graph	1.31	1	1	1
Balaban 11-cage	41.25	20.44	18.04	16
Gray graph	21.6	9	9	9
Nauru graph	9.6	4	4	4
Blanusa first snark graph	5.68	2.43	2.43	2
Pappus graph	7.2	3	3	3
Blanusa second snark graph	4.82	3.15	2.50	2
Brinkmann graph	4.49	2.14	1.97	1
Harborth graph	12.83	8.49	8.11	6
Perkel graph	5.52	3.79	1	1
Harries graph	28	12.82	10.71	10
Bucky ball	19.02	10.42	8.84	7
Harries-Wong graph	28	12.82	10.71	9
Robertson graph	3.91	1.82	1.77	1
Heawood graph	5.37	1	1	1
Cell 600	7.04	5.84	4.85	3
Cell 120	129.22	74.51	57.41	-
Hoffman graph	6.59	2	2	2
Sylvester graph	5.32	1	1	1
Coxeter graph	7.70	4	4	4
Holt graph	4.83	2.85	2.21	1
Szekeres snark graph	15.76	8.46	7.35	6
Desargues graph	8	2.5	2.5	2
Horton graph	38.4	16.89	16	14
Dejter graph	48.43	8	8	8
Tietze graph	3.54	1.87	1.87	1
Double star snark	9.29	5.36	4.37	4
Durer graph	3.40	2.24	2.18	2
Klein 3-regular Graph	17.09	9.80	7.29	7
Truncated tetrahedron	2.93	2.2	1.6	1
Dyck graph	12.8	4	4	4
Klein 7-regular graph	2.04	1	1	1
Tutte 12-cage	50.4	21	21	21
Ellingham-Horton 54-graph	21.6	9.92	9	8
Tutte-Coxeter graph	12	5	5	5
Ellingham-Horton 78-graph	31.2	13.73	13	11

Ljubljana graph	44.8	21.37	18.67	17
Tutte graph	15.21	8.17	7.17	6
F26A graph	10.4	5.10	3.61	3
Watkins snark graph	14.75	9.23	7.25	6
Flower snark	6.78	3.55	2.89	2
Markstroem graph	6.64	4.76	4.30	3
Wells graph	4.72	2	2	2
Folkman graph	8.24	2.5	2.5	2
Foster graph	36	15	15	15
McGee graph	7.32	4.13	3.0	2
Franklin graph	4.8	1.5	1.5	1
Hexahedron	3.2	1	1	1
Dodecahedron	4.52	3.24	2.36	2
Icosahedron	1.72	1	1	1
Brouwer-Haemers Graph	3.17	1	1	1

From Table 5.3, we observe that our bound holds with equality for some graphs, which gives rise to a regular partition of the matrix $A^3 - (\theta_s + \theta_{s+1} + \theta_d)A^2 + (\theta_d\theta_s + \theta_d\theta_{s+1} + \theta_s\theta_{s+1})A$, where A is the adjacency matrix of the graphs. The graphs are listed in Table 5.4.

5.7 Comparing Our Bound with the Bound of Fiol

Recall the polynomial given by Fiol [31] and its corresponding bound on the 3-independence number presented in Corollary 3.2.9. Recall that θ_i in Corollary 3.2.9 is the largest eigenvalue such that $\theta_i \leq -1$. Recall also that from Theorem 4.2.2, s is the largest index such that $\theta_s \geq -\frac{\theta_0^2+\theta_0\theta_d-\triangle}{\theta_0(\theta_d+1)}$, where $\triangle = \max_{u\in V}\{(A^3)_{uu}\}$. Let $\tau = -\frac{\theta_0^2+\theta_0\theta_d-\triangle}{\theta_0(\theta_d+1)}$. Note that $\triangle$ is $2n_t$ for a graph G that is at least 3-partially walk regular. Since $\triangle \leq \theta_0(\theta_0 - 1)$, we have that $\theta_s \geq \tau \geq -1$. In particular, if G is bipartite, then $\theta_s \geq 0$. If there exists an eigenvalue μ of G, where $\mu \in (\theta_i, \theta_s)$, then $\theta_{s+1} \geq \mu$ and $\theta_{i-1} \leq \mu$. Thus, $\theta_{i-1} \neq \theta_s$ (that is, $\theta_i \neq \theta_{s+1}$), and so these two bounds, Corollary 3.2.9 and Theorem 4.2.2, do not coincide.

Let us summarize the above discussion in the following proposition.

Proposition 5.7.1. Let $\tau = -\frac{\theta_0^2+\theta_0\theta_d-\triangle}{\theta_0(\theta_d+1)}$. The bound on the 3-independence number given in Corollary 3.2.9 is greater than the bound in Theorem 4.2.2 if and only if there exists an eigenvalue μ of G such that $\mu \in (-1, \tau)$.

Alternatively, if we take the polynomial $f(x)$ in Fiol's bound and take θ_i to be θ_{s+1}, then the polynomial is of the form $f(x) = B\,p(x) + C$ for some constants B and C, and $p(x)$ is our polynomial. So, the bounds resulting from $f(x)$ and $p(x)$ will coincide precisely when θ_i coincides with θ_{s+1}.

Table 5.4: Some named graphs in Sage that match our bound.

Graph	α_3
Cube Graph(8)	16
Moebius-Kantor graph	2
Gosset graph	1
Gray graph	9
Nauru graph	4
Pappus graph	3
Perkel graph	1
Heawood graph	1
Hoffman graph	2
Sylvester graph	1
Coxeter graph	4
Dejter graph	8
Dyck graph	4
Tutte 12-cage	21
Tutte-Coxeter graph	5
Wells graph	2
Foster graph	15
Hexahedron	1
Icosahedron	1
Brouwer-Haemers Graph	1

5.8 The k-Independence Number: A Polynomial for a General k

As noted in [2], Theorem 3.2.3 is interesting if one can come up with a good choice for the polynomial $p \in \mathbb{R}_k[x]$. So far there are optimal polynomials that minimize bound (3.2.1) from Theorem 3.2.3 for $k = 1, 2, 3$. It would be great to obtain a true optimal polynomial for a general $k \geq 4$, and hence an optimal bound for α_k of the form given in Theorem 3.2.1. Fiol [31] introduced the so called minor polynomials for this purpose. In [3], the authors propose the use of a Mixed Integer Programming (MILP) implementation which gives a polynomial that minimizes the bound. Closed form polynomials in terms of the eigenvalues of the graph is most desired. We don't have a closed form but in this section we propose a possible closed form polynomial.

5.8.1 For General k

Recall G is a regular graph on n vertices with the eigenvalues $\text{ev}(G) = \{\theta_0, \theta_1^{m_1}, \dots, \theta_d^{m_d}\}$, where $\theta_0 > \theta_1 > \cdots > \theta_d$.

It is easy to see that if $f(x) = p(x) - \lambda(p)$, then

$$\alpha_k \le n\frac{W(p) - \lambda(p)}{p(\theta_0) - \lambda(p)} = n\frac{W(f)}{f(\theta_0)}.$$

By analyzing the behavior of optimal polynomials for $k = 1, 2, 3$, we observe a pattern that can be generalized. Let us consider the specific cases.

- For $k = 1$, we have that $\lambda(p) = p(\theta_d)$ and an optimal polynomial is $p(x) = x$. Thus, $f(x) = x - \theta_d$ yields the same bound. Here $\lambda(f) = f(\theta_d) = 0$.

- For $k = 2$, we have that $\lambda(p) = p(\theta_i) = p(\theta_{i-1})$, where θ_i is the largest eigenvalue such that $\theta_i \le -1$. An optimal polynomial is $p(x) = x^2 - (\theta_i + \theta_{i+1})x$. As before, $f(x) = (x-\theta_i)(x-\theta_{i+1})$ yields the same bound and $\lambda(f) = f(\theta_i) = f(\theta_{i+1}) = 0$.

- For $k = 3$, we have that $\lambda(p) = p(\theta_d) = p(\theta_s) = p(\theta_{s+1})$ where θ_s is the least eigenvalue such that $\theta_s \ge -\frac{\theta_0^2 + \theta_0\theta_d - \triangle}{\theta_0(\theta_d + 1)}$. An optimal polynomial is $p(x) = x^3 - (\theta_s + \theta_{s+1} + \theta_d)x^2 + (\theta_d\theta_s + \theta_d\theta_{s+1} + \theta_s\theta_{s+1})x$. Similarly, the polynomial $f(x) = (x - \theta_d)(x - \theta_{s+1})(x - \theta_s)$ yields the same bound.

This observed pattern suggests that, in general, an optimal polynomial $p(x)$ has value $\lambda(p)$ at k distinct eigenvalues, occurring for some index set $I \subset \{1, \dots, d\}$ of size $|I| = k$ and $d \in I$ if k is odd. That is, $\lambda(p) = \prod_{i \in I} \theta_i = p(\theta_i)$ for $i \in I$. Alternatively, an optimal polynomial is of the form $f(x) = \prod_{i\in I}(x - \theta_i)$ where $\lambda(f) = f(\theta_i) = 0$ for all $i \in I$.

Fiol's minor polynomial formulation aligns with these observations. Fiol [31] in using the minor polynomial showed that an optimal polynomial $p(x)$ is of the form $\prod_{i\in I} \frac{x-\theta_i}{\theta_0-\theta_i}$, for some index set $I \subset \{1, \dots, d\}$ of size $|I| = k$ and $d \in I$ if k is odd. Our observation is consistent with Fiol's minor polynomials, which is a normalization of $f(x)$. The challenge lies in selecting the appropriate indices of the eigenvalues. One could try all possible indices and take the minimum, see Theorem 3.2.8. Abiad et al [3] would later used Linear programming to optimize these results. In keeping to the spirit of having a closed form formula, one can make some further observations about suitable indices.

Proposition 5.8.1. *Suppose p is an optimal polynomial of the above form with respect to the index set $I = \{i_1, i_2 \dots, i_k\}$ of size k such that $i_1 < i_2 < \cdots < i_k$. Then $i_{2r} = i_{2r-1} + 1$.*

Proof: Firstly, no $\lambda(p)$ occurs at a local minimum of $p(x)$. Otherwise, we would have a polynomial with $\lambda(p)$ occurring at fewer than k eigenvalues, contradicting our requirement. Therefore $p(x) - \lambda(p)$ changes sign at $x = \theta_i$ with $i \in I$.

Now, assume s is even, and $i_s > j > i_{s-1}$ with $j \notin I$. Then $\theta_{i_s} < \theta_j < \theta_{i_{s-1}}$ with $\lambda(p) = p(\theta_{i_s})$ and $\lambda(p) = p(\theta_{i_{s-1}})$. But then, this implies that $p(\theta_{i_s}) > p(\theta_j)$ and $p(\theta_{i_{s-1}}) > p(\theta_j)$, contradicting the fact that $\lambda(p)$ is the minimum value of p over all eigenvalues. ∎

Let us conclude by considering two examples from Fiol's work, the Johnson graph $J(14,7)$ and the Hamming graph $H(7,2)$, where the indices correspond to the zero (0) entries in [Table 1 and Table 2 in [31]]. The spectrum of $J(14,7)$ is

$$\text{ev}\, J(14,7) = \{49, 35^{13}, 23^{77}, 13^{273}, 5^{637}, -1^{1001}, -5^{1001}, -7^{429}\}$$

Below, we give $\lambda(p)$ for an optimal polynomial $p(x)$. We also give the corresponding alternate polynomial $f(x)$ and recall that $\lambda(f) = 0$ in each case.

- $k = 1$, we have $\lambda(p) = p(-7)$, and $f(x) = x + 7$
- $k = 2$, we have $\lambda(p) = p(-1) = p(5)$, and $f(x) = (x+1)(x-5)$.
- $k = 3$, we have $\lambda(p) = p(-7) = p(-1) = p(5)$, and $f(x) = (x+7)(x+1)(x-5)$
- $k = 4$, we have $\lambda(p) = p(-5) = p(-1) = p(5) = p(13)$, and $f(x) = (x+5)(x+1)(x-5)(x-13)$.
- $k = 5$, we have $\lambda(p) = p(-7) = p(-1) = p(5) = p(13) = p(23)$, and $f(x) = (x+7)(x+1)(x-5)(x-13)(x-23)$
- $k = 6$, we have $\lambda(p) = p(-7) = p(-5) = p(-1) = p(5) = p(13) = p(23)$, and $f(x) = (x+7)(x+5)(x+1)(x-5)(x-13)(x-23)$
- $k = 7$, we have $\lambda(p) = p(-7) = p(-5) = p(-1) = p(5) = p(13) = p(23) = p(35)$, and $f(x) = (x+7)(x+5)(x+1)(x-5)(x-13)(x-23)(x-35)$

We can do same for the Hamming graph $H(7,2)$. The spectrum of $H(7,2)$ is

$$\text{ev}\, H(7,2) = \{7, 5^7, 3^{21}, 1^{35}, -1^{35}, -3^{21}, -5^7, -7\}$$

- $k = 1$, we have $\lambda(p) = p(-7)$, and $f(x) = x + 7$
- $k = 2$, we have $\lambda(p) = p(-1) = p(1)$, and $f(x) = (x+1)(x-1)$.
- $k = 3$, we have $\lambda(p) = p(-7) = p(-1) = p(1)$, and $f(x) = (x+7)(x+1)(x-1)$

- $k = 4$, we have $\lambda(p) = p(-5) = p(-3) = p(1) = p(3)$, and $f(x) = (x+5)(x+3)(x-1)(x-3)$.
- $k = 5$, we have $\lambda(p) = p(-7) = p(-3) = p(-1) = p(1) = p(3)$, and $f(x) = (x+7)(x+3)(x+1)(x-1)(x-3)$
- $k = 6$, we have $\lambda(p) = p(-5) = p(-3) = p(-1) = p(1) = p(3) = p(5)$, and $f(x) = (x+5)(x+3)(x+1)(x-1)(x-3)(x-5)$
- $k = 7$, we have $\lambda(p) = p(-7) = p(-5) = p(-3) = p(-1) = p(1) = p(3) = p(5)$, and $f(x) = (x+7)(x+5)(x+3)(x+1)(x-1)(x-3)(x-5)$.

Chapter 6

Counting Closed Walks in Regular Trees: Exploring Combinatorial Structures with Catalan and Borel's Triangles

In determining the k-independence number of a graph using Theorem 3.2.1, a crucial factor is the knowledge of closed walks centered on vertices. However, for $k > 3$, calculating the number of such walks becomes challenging. To address this, we focus on graphs with a large girth, ideally at least the size of $k + 1$. By localizing around a vertex, we consider a regular tree. A finite regular graph with girth greater than $2n$ effectively acts as a tree locally, enabling us to leverage results from the enumeration of closed walks on an infinite regular tree.

Precisely, we investigate the question: What is the number of closed walks of length $2n$ that start and end at a vertex $v \in V(G)$ in an infinite δ-regular tree G, where $n \in \mathbb{N}$?

6.1 Introduction

Counting closed walks on a vertex in a regular tree has been a topic of interest, traditionally approached through generating functions. In this chapter, we present a new combinatorial approach to counting closed walks in an infinite δ-regular tree using Catalan's triangle and Borel's triangle. These two arrays of numbers, which have found applications in various fields of mathematics, provide alternative perspectives and shed light on the underlying combinatorial structures.

The generating function for the number of closed walks of length $2n$ starting and ending at a vertex in a regular tree was previously derived and studied extensively. McKay [58], Rowland et al. [63] and other researchers explored the generating function's properties and connections. The generating function was given [63] as

$$f_\delta(t) = \frac{2(\delta-1)}{\delta - 2 + \delta\sqrt{1-4(\delta-1)t^2}}.$$

Catalan's triangle, a classic combinatorial array, counts various objects such as Dyck paths, binary trees, and mountain ranges. Our result establishes a direct correspondence between the number of closed walks in a regular tree and the entries of Catalan's triangle. This combinatorial interpretation offers insights into the underlying structures of closed walks. Borel's triangle is an array of numbers closely related to the Catalan numbers. Borel's triangle has recently gained attention in studies of commutative algebra, combinatorics, discrete geometry, Cambrian Hopf algebras [17], quantum physics [51], and permutation patterns [62]. Cai and Yan [15] studied some classes of objects that are counted by Borel's triangle and characterized their combinatorial structures. In this chapter, we show how Borel's triangle and Catalan's triangle are involved in the well-known closed walk counting problem thereby showcasing another practical application of these two combinatorial structures. In particular, the number of closed walks centred on a vertex is a polynomial in δ with coefficients aligning with the terms of the Borel triangle.

6.2 Preliminaries and Problem Setup

In this section, we introduce some preliminary concepts and set up the problem of interest. We begin by recalling the properties of Catalan's triangle and Borel's triangle. The letter k in the rest of this document has no relation with the letter k in k-independence.

Catalan's triangle, denoted by $C_{n,k}$, counts the number of lattice paths in the coordinate plane from $(0,0)$ to (n,k) that do not go above the line $y = x$. The explicit formula for $C_{n,k}$ is given by

$$C_{n,k} = \frac{n-k+1}{n+1}\binom{n+k}{n}.$$

Catalan's triangles are the sequences $A009766$ on the On-line Encyclopedia of Integer Sequences (OEIS) [64]. The entries of $C_{n,k}$ for $0 \le n, k \le 7$ are in Table 6.1.

Borel's triangle, denoted by $B_{n,k}$, is derived from Catalan's triangle using an invertible transformation. The formula (see Cai and Yan [15]) for $B_{n,k}$ is given by

$$B_{n,k} = \sum_{s=k}^{n} \binom{s}{k} C_{n,s}. \tag{6.2.1}$$

Table 6.1: The entries of the Catalan triangle, $C_{n,k}$, for $0 \le n, k \le 7$.

$n\backslash k$	0	1	2	3	4	5	6	7
0	1							
1	1	1						
2	1	2	2					
3	1	3	5	5				
4	1	4	9	14	14			
5	1	5	14	28	42	42		
6	1	6	20	48	90	132	132	
7	1	7	27	75	165	297	429	429

Table 6.2: The entries of the Borel triangle, $B_{n,k}$, for $0 \le n, k \le 7$

$n\backslash k$	0	1	2	3	4	5	6	7
0	1							
1	2	1						
2	5	6	2					
3	14	28	20	5				
4	42	120	135	70	14			
5	132	495	770	616	252	42		
6	429	2002	4004	4368	2730	924	132	
7	1430	8008	19656	27300	23100	11880	3432	429

An explicit formula for $B_{n,k}$ is provided by Barry [7] as

$$B_{n,k} = \frac{1}{n}\binom{2n+2}{n-k}\binom{n+k}{n}.$$

Borel's triangles are the sequences $A234950$ on the On-line Encyclopedia of Integer Sequences (OEIS) [64]. The entries of $B_{n,k}$ for $0 \le n, k \le 7$ are in Table 6.2.

Now, let G be an infinite δ-regular tree. The results we present in this thesis can also be applied to finite δ-regular graphs of order m with girth greater than $2n$, where $n \in \mathbb{N}$. For the purpose of finding closed walks at vertex v, we assume that G is rooted at vertex v. Any closed walk from the root v can be represented as an RL-sequence, which is a sequence of moves away from the root (R) and towards the root (L).

Definition 6.2.1. *An RL-sequence is called* balanced *if it contains an equal number of R's and L's.*

Any closed walk must be balanced. Thus, there are no odd closed walks since they cannot be balanced. We further refine the notion of balanced RL-sequences by introducing the concept of legal sequences.

Definition 6.2.2. *A balanced RL-sequence is called* legal *if at any point in the sequence, the number of L's does not exceed the number of R's.*

Hence, closed walks from the root v can be represented as balanced legal RL-sequences. Notably, a balanced legal RL-sequence of length $2n$ can be viewed as a Dyck path of length $2n$ or semi-length n.

Definition 6.2.3. *A* component *of an RL-sequence S is formed when the sequence touches the root vertex v. The first component starts from the first R move from v to the first L that touches v. The second component starts from the second R move from v to the second L that touches v, and so on.*

The following lemma is immediate from the definition.

Lemma 6.2.4. *Every balanced legal RL-sequence can be expressed as a sequence of its components.* ∎

With these preliminary concepts established, we are now ready to proceed further.

6.3 Main Results

In this section, we present the main results. We first state an important lemma.

From this point forward, a sequence shall denote a balanced legal sequence. Let $\mathcal{S}_{n,k}$ be the set of RL-sequences of length $2n$ with exactly k components, and let $S_{n,k} = |\mathcal{S}_{n,k}|$.

Lemma 6.3.1. *Let $n, k \in \mathbb{Z}^+$ with $k \leq n$. The number of sequences of length $2n$ with exactly k components is equal to the number of sequences of length $2(n-1)$ with at least $k-1$ components. In other words,*

$$S_{n,k} = \sum_{j=k-1}^{n-1} S_{n-1,j}.$$

Proof: We define a deletion function f_i. The deletion function f_i removes the pair RL that forms the initial (R) and terminal (L) letters of the ith component of a sequence. We are proving more than needed. In fact, for the proof, it suffices to do f_1.

Let $\omega \in \mathcal{S}_{n,k}$. A sequence $\alpha \in \mathcal{S}_{n-1,j}$, for $k-1 \leq j \leq n-1$, can be achieved by applying a deletion function f_i to ω.

We note the following observations.

i. $f_i(\omega) \in \mathcal{S}_{n-1,k-1}$ if the ith component consists of only RL. Otherwise:

ii. $f_i(\omega) \in \mathcal{S}_{n-1,j}$, $k \leq j \leq n-1$.

We will now show that for fixed i, f_i is injective.

Suppose $\omega_1, \omega_2 \in \mathcal{S}_{n,k}$ and $\omega_1 = A_1 A_2 \dots A_k \neq B_1 B_2 \dots B_k = \omega_2$, where A_j and B_j are components for all $j \in [1, k]$, but $f_i(\omega_1) = f_i(\omega_2)$. Then, we have

$$f_i(\omega_1) = A_1 A_2 \dots A_{i-1} \bar{A}_i A_{i+1} \dots A_k,$$
$$f_i(\omega_2) = B_1 B_2 \dots B_{i-1} \bar{B}_i B_{i+1} \dots B_k,$$

where $\bar{A}_i$ and $\bar{B}_i$ are some legal sequences. So $f_i(\omega_1) = f_i(\omega_2)$ implies $A_j = B_j$ for all $j \in [1, k] \backslash \{i\}$ and $\bar{A}_i = \bar{B}_i$. We note that the deleted terms of component i in each of ω_1 and ω_2 are R and L. Thus, $A_i = R\bar{A}_i L$ and $B_i = R\bar{B}_i L$. But since $\bar{A}_i = \bar{B}_i$, then $A_i = B_i$ which necessarily implies $\omega_1 = \omega_2$. This proves the injectivity of f_i for a fixed i.

Now, we show that for i fixed, f_i is surjective.

Given $\alpha \in \mathcal{S}_{n-1,j}$, where $k-1 \leq j \leq n-1$, we can construct an $\omega \in \mathcal{S}_{n,k}$ as follows:

First, we decompose α into its components, say $\alpha = C_1 C_2 C_3 \dots C_j$. Now consider the components from i to the $(j-k+i)$th component of α, i.e., $C_i C_{i+1} \dots C_{j-k+i}$, and call it φ. We then place R and L in front and behind φ respectively, and call it C_i^*. Thus, $C_i^* = RC_i C_{i+1} \dots C_{j-k+i} L$. Note that C_i^* is a single component. We can then set $\omega = C_1 C_2 \dots C_{i-1} C_i^* \underbrace{C_{(j-k+i+1)} \dots C_j}_{k-i}$. Therefore, for every $\alpha = C_1 C_2 C_3 \dots C_j$, there exists an $\omega = C_1 C_2 \dots C_{i-1} C_i^* \underbrace{C_{(j-k+i+1)} \dots C_j}_{k-i}$ such that $f_i(\alpha) = f_i(C_1 C_2 \dots C_{i-1} C_i^* C_{(j-k+i+1)} \dots C_j) = C_1 C_2 C_3 \dots C_j$. Hence, there is a bijection $f_i : \mathcal{S}_{n,k} \to \cup_{j=k-1}^{n-1} \mathcal{S}_{n-1,j}$, which then implies the claim. ∎

Using Lemma 6.3.1, we have the following theorem.

Theorem 6.3.2. *Let G be an infinite δ-regular tree. The number of closed walks of length $2n$ at a vertex v of G is given by*

$$W_{2n} = \sum_{k=1}^{n} \left[\delta^k (\delta-1)^{n-k} \sum_{j \geq k-1} S_{n-1,j} \right]. \tag{6.3.1}$$

Proof: By Lemma 6.2.4, the closed walks of length $2n$ can be decomposed into balanced legal sequences with different numbers of components, specifically $k = 1, \dots, n$. In a sequence, an R move starting at v has δ possibilities, while an R move at any other vertex has $\delta - 1$ possibilities. However, an L move is completely determined since G is a tree. Hence, a sequence with k components has $\delta^k(\delta-1)^{n-k}$ possibilities. According to Lemma 6.3.1, there are $\delta^k(\delta-1)^{n-k}\sum_{j\geq k-1} S_{n-1,j}$ such sequences with k components. Since k runs from 1 to n, we have the desired result. ∎

Corollary 6.3.3. *Let G be a finite δ-regular graph of order m. Suppose G has girth greater than $2n \in \mathbb{Z}$. Then the number of closed walks of length $2n$ at a vertex v in G is given by W_{2n} as in Equation (6.3.1).* ∎

We note that for $n > 0$, $\sum_{j\geq 0} S_{n-1,j} = \sum_{j\geq 1} S_{n-1,j} = C_{n-1}$, the $(n-1)$th Catalan number. Therefore, the nth Catalan number, C_n, is the sum of the number of balanced sequences of length $2n$ with at least 1 component. We summarize this in the following corollary.

Corollary 6.3.4. *The nth Catalan number, C_n, for $n > 0$, is given by*

$$C_n = \sum_{j=1}^{n} S_{n,j} = \sum_{k=1}^{n} \sum_{j\geq k-1} S_{n-1,j}. \tag{6.3.2}$$

∎

The second equality in Equation (6.3.2) comes directly from using Lemma 6.3.1.

The following result by Lubotzky et al. [55] is a consequence of Theorem 6.3.2, and further discussion can be found in [24].

Corollary 6.3.5. *Let G be an infinite δ-regular tree. The number of walks of length $2n$ in G that start at vertex v and end at v for the first time is given by*

$$\begin{aligned} W_{2n} &= \delta(\delta-1)^{n-1}\sum_{j\geq 0} S_{n-1,j} \\ &= \delta(\delta-1)^{n-1}C_{n-1}. \end{aligned}$$

Proof: The result follows from the fact that such a walk contains just one component, $k = 1$. ∎

We can obtain a similar result if we seek closed walks that touch the vertex exactly twice, that is, have exactly two components.

Corollary 6.3.6. *Let G be an infinite δ-regular tree. The number of walks of length $2n$ in G that start at vertex v and end at v after touching it the second time is given by*

$$W_{2n} = \delta^2(\delta-1)^{n-2}C_{n-1}.$$

Proof: The result follows from the fact that such a walk contains two components, $k = 2$. Utilizing the fact that $\sum_{j\geq 0} S_{n-1,j} = \sum_{j\geq 1} S_{n-1,j} = C_{n-1}$ yields the desired result. ∎

We can delve further. The following result is due to Cai and Yan [15].

Theorem 6.3.7 (Cai and Yan [15])**.** *The entry $C_{n,k}$ of Catalan's triangle counts Dyck paths of semi-length $n+1$ that have k up-steps (or down-steps) not at ground level. Equivalently, it is the set of Dyck paths of semi-length $n+1$ with $n+1-k$ returns to the x-axis (not counting the starting point $(0,0)$).*

Thus, $C_{n,k}$ counts the RL sequences of length $2(n+1)$ with $n+1-k$ components. Similarly, $C_{n-1,n-k}$ counts the RL sequences of length $2n$ with k components. Consequently, there are $\delta^k(\delta-1)^{n-k}C_{n-1,n-k}$ closed walks of length $2n$ with k components (or that return to vertex v exactly k times). As k runs from 1 to n, we have the following result expressing the number of closed walks in terms of the Catalan's triangles.

Theorem 6.3.8. *Let G be an infinite δ-regular tree (or a finite δ-regular graph of order m with girth greater than $2n$). The number of closed walks of length $2n$ at vertex v of G is given by*

$$W_{2n} = \sum_{k=1}^{n} \delta^k(\delta-1)^{n-k}C_{n-1,n-k}. \tag{6.3.3}$$

where $C_{n,k}$ is the Catalan's triangle. ∎

By comparing Theorem 6.3.2 and Theorem 6.3.8, we can deduce another combinatorial interpretation of the $(n-1, n-k)$ entry of the Catalan's triangle.

Corollary 6.3.9. *In the Catalan's triangle, $C_{n-1,n-k}$ counts the number of RL sequences of length $2(n-1)$ with at least $k-1$ components. Equivalently, it counts Dyck paths of semi-length $n-1$ with at least $k-1$ returns to the x-axis (not counting the starting point $(0,0)$). That is,*

$$C_{n-1,n-k} = \sum_{j\geq k-1} S_{n-1,j}.$$

Corollary 6.3.10 (Cai and Yan [15]). *The entry $B_{n,k}$ of Borel's triangle counts the set of pairs (D, S) where D is a Dyck path of semi-length $n+1$ and S consists of k up-steps, none of which is at ground level.*

Recall from Equation 6.2.1 that we have

$$B_{n,k} = \sum_{s=k}^{n} \binom{s}{k} C_{n,s}.$$

Thus, we can express the number of closed walks at a vertex in terms of Borel's triangle as well.

Theorem 6.3.11. *Let G be an infinite δ-regular tree (or a finite δ-regular graph of order m with girth greater than $2n$). The number of closed walks of length $2n$ at vertex v of G is given by*

$$\begin{aligned} W_{2n} &= \sum_{\ell=1}^{n} (-1)^{n-\ell} B_{n-1,n-\ell}\, \delta^{\ell} \\ &= \sum_{\ell=0}^{n-1} (-1)^{\ell} B_{n-1,\ell}\, \delta^{n-\ell}, \end{aligned}$$

where $B_{n,k}$ is Borel's triangle.

Proof: Consider the coefficient of δ^{ℓ} in Equation (6.3.3). We have:

$$\begin{aligned} [\delta^{\ell}]W_{2n} &= [\delta^{\ell}] \sum_{k=1}^{n} \delta^{k} (\delta-1)^{n-k} C_{n-1,n-k} \\ &= [\delta^{\ell}] \sum_{k=1}^{\ell} \delta^{k} (\delta-1)^{n-k} C_{n-1,n-k} \\ &= [\delta^{\ell-k}] \sum_{k=1}^{\ell} (\delta-1)^{n-k} C_{n-1,n-k} \\ &= [\delta^{\ell-k}] \sum_{k=1}^{\ell} \sum_{i=0}^{n-k} \binom{n-k}{i} \delta^{n-k-i} (-1)^{i} C_{n-1,n-k} \\ &= \sum_{k=1}^{\ell} \binom{n-k}{n-\ell} (-1)^{n-\ell} C_{n-1,n-k} \\ &= (-1)^{n-\ell} \sum_{k=1}^{\ell} \binom{n-k}{n-\ell} C_{n-1,n-k} \end{aligned}$$

$$= (-1)^{n-\ell} \sum_{s=n-\ell}^{n-1} \binom{s}{n-\ell} C_{n-1,s}$$
$$= (-1)^{n-\ell} B_{n-1,n-\ell}.$$

Since ℓ runs from 1 through n, we have:

$$W_{2n} = \sum_{\ell=1}^{n} (-1)^{n-\ell} B_{n-1,n-\ell} \delta^{\ell}.$$

∎

We can indeed rephrase this in a more revealing manner. If one wants to know the number of closed walks of length $2n$ at a vertex of G, one needs to only form a degree n polynomial in δ with no constant term. The coefficients of this polynomial are the terms of the Borel triangle $B_{n-1,k}$.

Corollary 6.3.12. *Let G be an infinite δ-regular tree, or a finite δ-regular graph of order m with girth greater than $2n$. Then, the number of closed walks W_{2n} of length $2n$ at a vertex v of G is a polynomial in δ of degree n with integer coefficients that alternate in sign. Moreover, the smallest power of δ occurring is 1, and the coefficients are the terms within the Borel triangle $B_{n-1,k}$.*

6.4 Examples

Table 6.3 illustrates the number of closed walks of length $2n$ centered at a vertex $v \in G$, where G is a δ-regular infinite tree or a finite δ-regular graph of order m with girth greater than $2n$.

In each section, the values in the columns represent entries from the Catalan triangle, providing insights into the enumeration of closed walks using Catalan triangle. The sum row labeled W_{2n} contains coefficients corresponding to sequences from the Borel triangles, providing an alternate perspective of these walks.

Table 6.3: Closed walks of different lengths in a δ-regular graph.

For length 2	
	$\delta \times \mathbf{1}$
$W_2 =$	δ
For length 4	
	$\delta^2 \times \mathbf{1}$
	$\delta(\delta-1) \times \mathbf{1}$
$W_4 =$	$\mathbf{2}\delta^{\mathbf{2}} - \delta$
For length 6	
	$\delta^3 \times \mathbf{1}$
	$\delta^2(\delta-1) \times \mathbf{2}$
	$\delta(\delta-1)^2 \times \mathbf{2}$
$W_6 =$	$\mathbf{5}\delta^{\mathbf{3}} - \mathbf{6}\delta^{\mathbf{2}} + \mathbf{2}\delta$
For length 8	
	$\delta^4 \times \mathbf{1}$
	$\delta^3(\delta-1) \times \mathbf{3}$
	$\delta^2(\delta-1)^2 \times \mathbf{5}$
	$\delta(\delta-1)^3 \times \mathbf{5}$
$W_8 =$	$\mathbf{14}\delta^{\mathbf{4}} - \mathbf{28}\delta^{\mathbf{3}} + \mathbf{20}\delta^{\mathbf{2}} - \mathbf{5}\delta$
For length 10	
	$\delta^5 \times \mathbf{1}$
	$\delta^4(\delta-1) \times \mathbf{4}$
	$\delta^3(\delta-1)^2 \times \mathbf{9}$
	$\delta^2(\delta-1)^3 \times \mathbf{14}$
	$\delta(\delta-1)^4 \times \mathbf{14}$
$W_{10} =$	$\mathbf{42}\delta^{\mathbf{5}} - \mathbf{120}\delta^{\mathbf{4}} + \mathbf{135}\delta^{\mathbf{3}} - \mathbf{70}\delta^{\mathbf{2}} + \mathbf{14}\delta$
For length 12	
	$\delta^6 \times \mathbf{1}$
	$\delta^5(\delta-1) \times \mathbf{5}$
	$\delta^4(\delta-1)^2 \times \mathbf{14}$
	$\delta^3(\delta-1)^3 \times \mathbf{28}$
	$\delta^2(\delta-1)^4 \times \mathbf{42}$
	$\delta(\delta-1)^5 \times \mathbf{42}$
$W_{12} =$	$\mathbf{132}\delta^{\mathbf{6}} - \mathbf{495}\delta^{\mathbf{5}} + \mathbf{770}\delta^{\mathbf{4}} - \mathbf{616}\delta^{\mathbf{3}} + \mathbf{252}\delta^{\mathbf{2}} - \mathbf{42}\delta$

Chapter 7

Connectivity and Graph Toughness

In this chapter, we shift our focus towards closely related themes: the connectivity and toughness of graphs. We present a slight improvement on the bound on the vertex connectivity of regular graphs given by Krivelevich and Sudakov [50]. We also give some general and spectral bounds on graph toughness and address a Laplacian toughness conjecture proposed by Haemers. We confirm this conjecture for some graphs.

7.1 Vertex Connectivity in d-Regular Graphs

In this section, we delve into the study of vertex connectivity in d-regular graphs, presenting advancements in understanding this concept.

Consider a d-regular graph G with adjacency eigenvalues $d = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Let $\lambda = \max\{\lambda_2, |\lambda_n|\}$. This λ value represents the maximum magnitude of eigenvalues, excluding the largest one. Our primary focus lies in exploring the vertex connectivity of graph G.

Vertex connectivity κ offers valuable insights into the structural properties and robustness of the graph, revealing the minimal number of vertices required to disconnect it.

Notably, Fiedler [28] established the bound $\kappa \geq d - \lambda_2$, while Krivelevich and Sudakov [50] made improvements within a specific range by leveraging the expander mixing lemma.

A graph G is an (n, d, λ)-graph if it is d-regular, has n vertices and $\lambda = \max\{\lambda_2, |\lambda_n|\}$.

Theorem 7.1.1. *(Krivelevich and Sudakov [50]) Let G be an (n, d, λ)-graph with $d \leq n/2$. Then the vertex connectivity of G satisfies*

$$\kappa \geq d - 36\lambda^2/d. \tag{7.1.1}$$

Cioabă and Gu [20] have introduced a condition on the second eigenvalue λ_2 that guarantees a vertex connectivity κ greater than 2, thus improving slightly upon the previous results of Krivelevich and Sudakov, as well as Fiedler.

Theorem 7.1.2. *(Cioabă and Gu [20]) For any connected d-regular graph G with $d > 3$, if*

$$\lambda_2 < \begin{cases} \frac{d-2+\sqrt{d^2+12}}{2} & \text{if } d \text{ is even} \\ \frac{d-2+\sqrt{d^2+8}}{2} & \text{if } d \text{ is odd} \end{cases} \tag{7.1.2}$$

then $\kappa \geq 2$.

We here establish a further generalization and improvement on the lower bound of vertex connectivity by Krivelevich and Sudakov, also by utilizing the Expander Mixing Lemma. The Expander Mixing Lemma, originally formulated by Alon and Chung [5], provides a powerful tool for analyzing graph expansion properties. We state the Expander Mixing Lemma.

Theorem 7.1.3. *(Expander Mixing Lemma) Let G be a d-regular graph on n vertices. Let $d = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of G. Denote $\lambda = \max\{\lambda_2, |\lambda_n|\}$. Then for every two subsets $A, B \subset V$,*

$$\left| e(A,B) - \frac{d|A||B|}{n} \right| \leq \lambda \sqrt{|A||B| \left(1 - \frac{|A|}{n}\right)\left(1 - \frac{|B|}{n}\right)}, \tag{7.1.3}$$

where $e(A,B) = |E(A,B)|$ is the number of edges $E(A,B)$ with one endpoint in A and the other endpoint in B.

Using the Expander Mixing Lemma, and inspired by the approach of Krivelevich and Sudakov, we establish the following improved bound:

Theorem 7.1.4. *Let G be an (n, d, λ)-graph with $d \leq n/2$. Then the vertex connectivity of G satisfies*

$$\kappa \geq d - 4\left(\frac{d+\lambda}{d-3\lambda}\right)^2 \lambda^2/d. \tag{7.1.4}$$

Proof: We can assume $\lambda \leq (\frac{-5+\sqrt{33}}{4})d$ since otherwise $\kappa \leq 0$ and there is nothing to prove. Suppose there exists a subset $S \subset V$ with size less than $d - 4\left(\frac{d+\lambda}{d-3\lambda}\right)^2 \frac{\lambda^2}{d}$ such that the induced subgraph $G[V-S]$ is disconnected. Let U be the set of vertices in the smallest component of $G[V-S]$, and let $W = V - (S \cup U)$, then it follows that $|U| \leq |W|$. Since there are no edges between U and W, we have $e(U,W) = 0$. Moreover, since all neighbors of a vertex in U are contained in $S \cup U$, we have

$|U|+|S|>d$, which implies $|U| \geq 4\left(\frac{d+\lambda}{d-3\lambda}\right)^2 \frac{\lambda^2}{d}$. By applying the Expander Mixing Lemma (Theorem 7.1.3), we obtain the following inequality:

$$\frac{d|U||W|}{n} \leq \lambda \sqrt{|U||W|\left(1-\frac{|U|}{n}\right)\left(1-\frac{|W|}{n}\right)}$$

which implies

$$d^2|U|^2|W|^2 \leq \lambda^2 |U||W|\left(n-|U|\right)\left(n-|W|\right)$$

and we have

$$|U||W| \leq \frac{\lambda^2}{d^2}\left(n-|U|\right)\left(n-|W|\right).$$

It follows that

$$|U|^2 \leq |U||W| \leq \frac{\lambda^2}{d^2}\left(n-|U|\right)\left(n-|W|\right) \leq \frac{\lambda^2}{d^2}\left(n-|U|\right)^2$$

and

$$|U| \leq \frac{\lambda}{d}\left(n-|U|\right).$$

Hence

$$|U| \leq \frac{\lambda n}{d+\lambda}.$$

Next, using the Expander Mixing Lemma (Theorem 7.1.3) again, we can derive an upper bound on the number of edges spanned by U:

$$\left|e(U,U)-\frac{d|U||U|}{n}\right| \leq \lambda \sqrt{|U|^2\left(1-\frac{|U|}{n}\right)^2}.$$

It follows that

$$2e(U) \leq \lambda |U|\left(1-\frac{|U|}{n}\right)+\frac{d}{n}|U|^2$$

and

$$\begin{aligned} e(U) &\leq \frac{\lambda}{2}|U|-\frac{\lambda}{2n}|U|^2+\frac{d}{2n}|U|^2 \\ &= \frac{\lambda}{2}|U|+\left(\frac{d-\lambda}{2n}\right)|U|^2 \end{aligned}$$

$$\leq \frac{\lambda}{2}|U| + \left(\frac{d-\lambda}{2n}\right)\frac{\lambda n}{d+\lambda}|U|$$
$$= \left(\frac{\lambda d}{d+\lambda}\right)|U|.$$

Since the degree of every vertex in U is d, it follows that:

$$e(U,S) \geq d|U| - 2e(U) > d|U| - 2\left(\frac{\lambda d}{d+\lambda}\right)|U| = \left(\frac{d-\lambda}{d+\lambda}\right)d|U|. \qquad (7.1.5)$$

On the other hand, by applying the Expander Mixing Lemma (Theorem 7.1.3), and considering that $|S| < d$, $d \leq n/2$, and $|U| \geq 4\left(\frac{d+\lambda}{d-3\lambda}\right)^2\frac{\lambda^2}{d}$, we can obtain the following inequality:

$$\begin{aligned} e(U,S) &\leq \frac{d|U||S|}{n} + \lambda\sqrt{|U||S|} \\ &< \frac{d}{n}d|U| + \lambda\sqrt{d|U|} \\ &\leq \frac{d}{2}|U| + \lambda\sqrt{d}\frac{|U|}{\sqrt{|U|}} \\ &\leq \frac{d}{2}|U| + \frac{\lambda\sqrt{d}|U|}{2\left(\frac{d+\lambda}{d-3\lambda}\right)\lambda/\sqrt{d}} \\ &= \frac{d}{2}|U| + \frac{d(d-3\lambda)|U|}{2\left(d+\lambda\right)} \\ &= \left(\frac{d-\lambda}{d+\lambda}\right)d|U|, \end{aligned}$$

which contradicts Equation (7.1.5).

Therefore, we have shown that there does not exist a subset $S \subset V$ of size less than $d - 4\left(\frac{d+\lambda}{d-3\lambda}\right)^2\frac{\lambda^2}{d}$ such that the induced subgraph $G[V-S]$ is disconnected. Consequently, the vertex connectivity κ of G satisfies $\kappa \geq d - 4\left(\frac{d+\lambda}{d-3\lambda}\right)^2\frac{\lambda^2}{d}$. ∎

Consider the case when $\lambda = \lambda_2$. Then by simplifying $36(\lambda_2)^2/d < \lambda_2$, we conclude that Krivelevich and Sudakov's bound (7.1.1) improves Fiedler's bound when $\lambda_2 < \frac{d}{36}$. Similarly, the new bound (7.1.4) derived in this thesis further improves Krivelevich and Sudakov's bound (7.1.1). It can be verified that the bound (7.1.4) improves Fiedler's bound when $\lambda_2 < \frac{d}{10}$. Therefore, the new bound (7.1.4) presents an enhancement over both Fiedler's bound and Krivelevich and Sudakov's bound, providing tighter constraints on the vertex connectivity κ of the d-regular graph G when $\lambda_2 < \frac{d}{10}$.

7.2 Graph Toughness

The concept of toughness of a graph defined below, was introduced by Chvátal in 1973, and has since led to much research, most of which are based on conjectures in his paper [19]. The toughness of a graph is closely related to several graph properties including Hamiltonicity, connectivity, and also to spanning trees, graph factors, among others.

Definition 7.2.1. *Let G be a connected graph. The toughness $t(G)$ of G is defined by*

$$t(G) = \min\left\{\frac{|S|}{c(G-S)} : S \text{ is a vertex cut of } G\right\}, \tag{7.2.1}$$

and $c(G-S)$ (or simply c) is the number of components of $G-S$.

A graph G is r-tough if $t(G) \geq r$ for a non negative $r \in \mathbb{R}$. That is, $|S| \geq rc(G-S)$ for every vertex cut S of G. If a graph is r-tough, an implication, by setting $c = 2$, is that any removal of a set of $2r-1$ vertices from the graph will not disconnect the graph. In other words, every r-tough graph is $2r$-vertex connected.

7.2.1 Spectral and General Bounds on Graph Toughness

Suppose G is a connected d-regular graph with adjacency eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and define $\lambda = \max\{\lambda_2, |\lambda_n|\}$. Similarly, for a connected graph G (not necessarily regular) with an order of n, we will denote its minimum degree as δ, its maximum degree as Δ, and its Laplacian eigenvalues as $0 = \mu_1 \leq \mu_2 \leq \cdots \leq \mu_n$.

Alon [4] was the first to study the lower bound of the toughness of a graph using the eigenvalues of the graph. Alon proved in [4] that

$$t(G) > \frac{1}{3}\Big(\frac{d^2}{d\lambda + \lambda^2} - 1\Big).$$

In 1995, Brouwer [11] proved a better bound $t(G) > \frac{d}{\lambda} - 2$ using interlacing, and conjectured that $t(G) > \frac{d}{\lambda} - 1$. His conjecture was proved by Gu [37] in 2020 using the Expander Mixing Lemma. Haemers conjectured the following lower bound, which would improve upon both of these bounds.

Conjecture 7.2.2 (Haemers)**.** Let G be a connected graph of order n with minimum degree δ and Laplacian eigenvalues $0 = \mu_1 \leq \mu_2 \leq \cdots \leq \mu_n$. Then the toughness $t(G)$ of G satisfies

$$t(G) \geq \frac{\mu_2}{\mu_n - \delta}. \tag{7.2.2}$$

Recall that if G is d-regular then $L = dI - A$. Thus if G is d-regular with adjacency eigenvalues $d = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, then $\mu_n = d - \lambda_n$ and $\mu_2 = d - \lambda_2$ and the conjectured lower bound (7.2.2) becomes

$$t(G) \geq \frac{d - \lambda_2}{-\lambda_n}, \tag{7.2.3}$$

which is stronger than Brouwer's conjecture. In [38], Gu and Haemers supported Conjecture 7.2.2 by showing it is true for some special cases.

We shall need the following relation. If κ and κ' are respectively the vertex connectivity and the edge connectivity of G, then

$$\mu_2 \leq \kappa \leq \kappa' \leq \delta. \tag{7.2.4}$$

For every disconnecting set S we have $|S| \geq \kappa$. By taking a vertex from each of the c components of $G - S$, we have an independent set in G. Hence $c(G - S) \leq \alpha$, where α is the independence number of G. Thus we have the following.

Theorem 7.2.3 (Chvátal [19])**.** *Let G be a graph with vertex connectivity κ with an independence number α. Then*

$$t(G) \geq \frac{\kappa}{\alpha}. \tag{7.2.5}$$

For a disconnecting set S, each connected component H_i of $G - S$ has at least κ' edges connecting it to S. Thus, in the case of a d-regular graph G, we have the inequality $\kappa' c \leq |S|d$. This leads to a bound on toughness of regular graphs in terms of the edge connectivity of the graph.

Theorem 7.2.4 (Cioabă and Gu [20])**.** *Let G be a connected d-regular graph with edge connectivity κ'. Then*

$$t(G) \geq \frac{\kappa'}{d}. \tag{7.2.6}$$

We recall the following bounds on the independence number of a graph.

Theorem 7.2.5 (Godsil and Newman [34], Lu, Liu and Tian [54])**.** *Let G be a graph with an independence number α. Then*

$$\alpha \leq \frac{\mu_n - \delta}{\mu_n} n. \tag{7.2.7}$$

Proof: Let U be an independent set of size α in G and let a be the number of edges between vertex set U and its complement $V \backslash U$. Define vector $\mathbf{v}$ by:

$$v_j = \begin{cases} n - \alpha & j \in U \\ -\alpha & j \in V \backslash U. \end{cases}$$

Then $\mathbf{v}^T\mathbf{v} = (n-\alpha)^2\alpha + (-\alpha)^2(n-\alpha) = \alpha n(n-\alpha)$ and $\mathbf{v}^T L\mathbf{v} = a(n-\alpha+\alpha)^2 = an^2$. Observe that $\mathbf{v}$ is orthogonal to the $\mathbf{1}$ vector, thus using the Rayleigh quotient, Corollary 2.3.4, and the fact that $a \geq \alpha\delta$, we get the following:

$$\mu_n \geq \frac{\mathbf{v}^T L\mathbf{v}}{\mathbf{v}^T\mathbf{v}} = \frac{an^2}{\alpha n(n-\alpha)} \geq \frac{n\alpha\delta}{\alpha(n-\alpha)} = \frac{n\delta}{(n-\alpha)},$$

from which we obtain the desired bound. ∎

We present the next independence bound.

Theorem 7.2.6 (O, Shi and Taoqiu [60])**.** *Let G be a graph with an independence number α. Then*

$$\alpha \leq \frac{\Delta}{\Delta+\delta}n. \tag{7.2.8}$$

We briefly state how these two independence bounds, Equations (7.2.7) and (7.2.8) are comparable. One can easily verify that (7.2.7) is stronger than (7.2.8) if and only if $\mu_n < \delta + \Delta$. Take for instance the path graph, P_n. It has $\mu_n = 4$, $\delta = 1$ and $\Delta = 2$, so $\mu_n = 4 > 1 + 2 = \delta + \Delta$. Thus for the path graph Theorem 7.2.6 gives a stronger bound than Theorem 7.2.5. Consider also the Petersen graph, it has $\mu_n = 5, \delta = \Delta = 3$, so $\mu_n = 5 < 3 + 3 = \delta + \Delta$. Thus Theorem 7.2.5 gives a stronger bound than Theorem 7.2.6 for the Petersen graph. The two bounds coincide for instance in the case of the complete bipartite graph $K_{a,b}$ since $\mu_n = a+b = \delta+\Delta$.

Conjecture 7.2.2 was shown to hold for the following.

Proposition 7.2.7 (Gu and Haemers [38])**.** *Let $S \subset V$ be such that $t(G) = |S|/c(G-S)$. Suppose all connected components of $G-S$ are singletons (i.e. $n-|S| = c(G-S)$), then*

$$t(G) \geq \frac{\mu_2}{\mu_n - \delta}.$$

Proof: If $n-|S| = c$, then $V\backslash S$ is an independent set of G. By use of Theorem 7.2.5 and (7.2.4) we have

$$t(G) = \frac{|S|}{c} \geq \frac{n-c}{c} = \frac{n}{c} - 1 \geq \frac{\mu_n}{\mu_n - \delta} - 1 = \frac{\delta}{\mu_n - \delta} \geq \frac{\mu_2}{\mu_n - \delta}.$$

∎

Gu and Haemers also proved the following.

Theorem 7.2.8 (Gu and Haemers[38])**.** *The toughness of a graph G satisfies the following.*

$$t(G) \geq \frac{\mu_n \mu_2}{n(\mu_n - \delta)}, \tag{7.2.9}$$

$$t(G) \geq \frac{\mu_2}{\mu_n - \mu_2}. \tag{7.2.10}$$

Using Equations (7.2.7) and (7.2.4), we see that Equation (7.2.9) is an immediate consequence of Theorem 7.2.3. Since $\mu_n \leq n$ and $\mu_2 \leq \delta$, the conjectured bound implies (7.2.9) and (7.2.10). Moreover, Equation (7.2.10) coincides with Conjecture 7.2.2 when $\mu_2 = \delta$. Similarly, Equation (7.2.9) coincides with Conjecture 7.2.2 when $\mu_n = n$, that is, if the complement of G is disconnected.

The *join* of two graphs H and F, denoted by $H \vee F$, is the graph obtained from H and F by connecting each vertex of H to every vertex of F. Thus the complement of $H \vee F$ is disconnected. The following is then immediate.

Corollary 7.2.9. *If $G \cong H \vee F$, where H and F are graphs, then Conjecture 7.2.2 is true for G.*

Example 7.2.10. The conjecture is true for the wheel graph W_{n+1} since $W_{n+1} \cong K_1 \vee C_n$, where K_1 is the complete graph on 1 vertex and C_n is the cycle graph on n vertices. It also holds for the complete k-partite graph $K_{n_1,n_2,...,n_k}$ which is the graph join of empty graphs on $n_1, n_2, ..., n_k$ vertices. In fact, Gu and Haemers showed Conjecture 7.2.2 is tight for $K_{n_1,n_2,...,n_k}$ in [38].

A graph is *maximally connected* if its connectivity equals its minimum degree. We have the following toughness bounds.

Theorem 7.2.11. *Suppose G is a maximally connected graph. Then*

$$t(G) \geq \frac{\delta}{\Delta n}(\Delta + \delta) \tag{7.2.11}$$

$$t(G) \geq \frac{\delta \mu_n}{n(\mu_n - \delta)}. \tag{7.2.12}$$

Proof: Since G is maximally connected, we have $s \geq \kappa = \delta$, where $s = |S|$ is the size of a disconnecting set S. Now taking exactly one vertex from each of the components of $G-S$, we obtained an independent set of size c. Thus by Theorem 7.2.6 we obtain $c \leq \frac{\Delta}{\Delta+\delta} n$. So we have

$$t(G) = \frac{s}{c} \geq \frac{\delta}{c} \geq \frac{\delta}{\Delta n}(\Delta + \delta).$$

Similarly, by Theorem 7.2.5 we have $c \le \frac{\mu_n - \delta}{\mu_n} n$. Thus, we obtain

$$t(G) = \frac{s}{c} \ge \frac{\delta}{c} \ge \frac{\delta \mu_n}{n(\mu_n - \delta)}$$

as desired. ∎

We provide a quick comparison of how these bounds perform on the Petersen graph. To recall, the Petersen graph is 3-regular, consisting of 10 vertices, with $\mu_n = 5$ and $\mu_2 = 2$. It has toughness equal to $\frac{4}{3}$. A straightforward verification of the conjecture in Equation (7.2.2) yields a bound of 1, whereas Equation (7.2.12) gives $\frac{3}{4}$. Equation (7.2.10) yields $\frac{2}{3}$, Equation (7.2.11) results in $\frac{3}{5}$, while Equation (7.2.9) yields $\frac{1}{2}$.

We also have the following bound.

Theorem 7.2.12. *Let G be a graph with minimum degree δ. Let $S \subset V$ be such that $G - S$ is disconnected. Let X and Y be disjoint vertex subsets of $V \backslash S$ with no edges between X and Y such that $X \cup Y = V \backslash S$ and $|X| \le |Y|$. If*

$$|S| \ge \frac{2\mu_2}{\mu_n - \delta}|X|, \tag{7.2.13}$$

then the toughness of the graph G satisfies the following.

$$t(G) \ge \frac{\mu_2}{\mu_n - \delta}. \tag{7.2.14}$$

Proof:

Let $V_1, \ldots, V_c$ denote the vertex sets of the c components of $G - S$. Without loss of generality, suppose that $|V_1| \le |V_2| \le \cdots \le |V_c|$. The bound was shown to hold in Proposition 7.2.7 if $V_1, \ldots, V_c$ are singletons. Thus, we may assume that $n - |S| \ge c + 1$. It was shown in [38] that $V_1, V_2, \ldots, V_c$ can be partitioned into two sets X and Y such that $|Y| \ge |X| \ge c/2$. For completeness, we write the proof again. If c is even, we can simply define $X = \cup_{1 \le i \le \lfloor c/2 \rfloor} V_i$ and $Y = (V \backslash S) \backslash X$. Now we assume c is odd. If $|V_{(c-1)/2}| \ge 2$, then define $X = \cup_{1 \le i \le (c-1)/2} V_i$ and $Y = (V \backslash S) \backslash X$ as needed.

The remaining case is $|V_1| = \cdots = |V_{(c-1)/2}| = 1$. We can define $X = \cup_{1 \le i \le (c+1)/2} V_i$ and $Y = (V \backslash S) \backslash X$, and we need to show that $|Y| \ge |X| \ge c/2$. If $|V_{(c+1)/2}| = 1$, then $|X| = \frac{c+1}{2}$ and $|Y| = n - |S| - |X| \ge \frac{c+1}{2}$, since $n - |S| \ge c + 1$. If $|V_{(c+1)/2}| \ge 2$, then $|X| = \frac{c-1}{2} + |V_{(c+1)/2}| \ge \frac{c-1}{2} + 2 > \frac{c}{2}$ and $|Y| = \sum_{i > (c+1)/2} |V_i| \ge 2\frac{c-1}{2} = c - 1 \ge c/2$. Switch X and Y whenever needed to get $|Y| \ge |X|$. It follows that $c \le 2|X|$. Thus, by (7.2.13), we have

$$t(G) = \frac{|S|}{c} \ge \frac{2\mu_2}{\mu_n - \delta}\frac{|X|}{c} \ge \frac{\mu_2}{\mu_n - \delta}. \tag{7.2.15}$$

■

While hypothesis (7.2.13) has been verified for several graphs, including the Petersen graph, establishing its validity for all graphs remains an open challenge. A weaker version of hypothesis (7.2.13), given as $|S| \geq \dfrac{2\mu_2}{\mu_n - \mu_2}|X|$, was successfully demonstrated in [38]. This weaker form together with the fact that $c \leq 2|X|$ led to the derivation of the bound presented in Equation (7.2.10).

Proposition 7.2.13. *Let G be a d-regular bipartite graph. Then Conjecture 7.2.2 holds for G. That is,*

$$t(G) \geq \frac{\mu_2}{\mu_n - d}. \tag{7.2.16}$$

Proof: We have that $\kappa' \geq \mu_2$ from (7.2.4). Moreover, since G is regular bipartite, we have $\mu_n = 2d$. Thus $\mu_n - \delta = 2d - d = d$. Hence, using Equation 7.2.6, we have $t(G) \geq \frac{\kappa'}{d} \geq \frac{\mu_2}{\mu_n - \delta}$ as desired. ■

Lemma 7.2.14 (Grone and Merris [36])**.** *Let G be a graph with a maximum degree Δ. The following bound holds:*

$$\Delta \leq \mu_n - 1. \tag{7.2.17}$$

Bound (7.2.17) is proved in [[36], Corollary 2].

Proposition 7.2.15. *Let G be a graph with a maximum degree Δ. Then the toughness of G satisfies the following.*

$$t(G) \geq \frac{1}{\Delta - 1 + \frac{1}{s}}, \tag{7.2.18}$$

where s is the size of a disconnecting set.

Bound (7.2.18) in Proposition 7.2.15 is uniformly sharper than the bound $t(G) \geq \frac{1}{\Delta}$ proved in [46]. We give the proof of Proposition 7.2.15 below.

Proof: (of 7.2.15)

Let S be a vertex cut of G such that $t(G) = \frac{|S|}{c(G-V)} = \frac{s}{c}$. Then clearly $c \leq s\Delta$. But since G is connected, there were at least $s-1$ edges connecting vertices in S with each other, or vertices in $V \backslash S$ with each other, or a combination of both. Therefore, $c \leq s\Delta - (s-1)$. Thus, the toughness is at least $\frac{s}{s\Delta - (s-1)}$, as desired. ■

Let us consider the toughness of a tree graph T with n vertices and maximum degree Δ. We show that the Conjecture 7.2.2 is true for a tree, but first, we determine the toughness $t(T)$ of the tree.

Proposition 7.2.16. *The toughness of a tree T with a vertex of maximum degree Δ is given by*

$$t(T) = \frac{1}{\Delta}. \tag{7.2.19}$$

Proof: Let $S = \{v\}$ where v is a vertex in T with maximum degree Δ. Since T is a tree, removing the vertex set S results in $c(T - S) = \Delta$ connected components.

To show the optimality of the chosen vertex set S, consider an alternative disconnecting set S' of size $|S'| > 1$. Then $c(G - S') < \sum_{j \in S'} \deg(j)$. So $\frac{c(G - S')}{|S'|} <$ average degree $< \Delta$. Thus, we have $\frac{|S'|}{c(G - S')} > \frac{1}{\Delta}$.

Consequently, for any tree T with maximum degree Δ, the toughness is bounded below by $\frac{1}{\Delta}$. By selecting a vertex with maximum degree, we achieve the optimal toughness, yielding $t(T) = \frac{1}{\Delta}$. ∎

The following is then immediate from the above proof.

Proposition 7.2.17. *The toughness $t(G)$ of a graph G is $t(G) = 1/\Delta$ if and only if there is an induced star where the central Δ-vertex is a cut-vertex.*

Now we verify Conjecture 7.2.2 for trees.

Proposition 7.2.18. *Conjecture 7.2.2 is true for a tree T. In particular,*

$$t(T) \geq \frac{\delta}{\mu_n - \delta}. \tag{7.2.20}$$

Proof: Recall from Proposition 7.2.16 that $t(T) = 1/\Delta$, where Δ is the maximum degree in T. Note also that from bound (7.2.17), we have $\Delta \leq \mu_n - 1 = \mu_n - \delta$. Now, since every tree has a vertex of degree 1 and $\mu_2 \leq \kappa \leq \delta$, we have $1 = \delta \geq \kappa \geq \mu_2$. Therefore, we have

$$t(T) = \frac{1}{\Delta} \geq \frac{1}{\mu_n - \delta} = \frac{\delta}{\mu_n - \delta} \geq \frac{\mu_2}{\mu_n - \delta}, \tag{7.2.21}$$

confirming the conjecture for trees. ∎

Using a similar approach, we prove the conjecture is true for graphs with at least one leaf.

Proposition 7.2.19. *Conjecture 7.2.2 is true for a graph G with at least one leaf. In particular,*

$$t(G) \geq \frac{\delta}{\mu_n - \delta}. \tag{7.2.22}$$

Proof: Since G has a leaf and $\mu_2 \leq \kappa \leq \delta$, we have $1 = \delta \geq \kappa \geq \mu_2$. From bound (7.2.17), we have $\Delta \leq \mu_n - 1 = \mu_n - \delta$. Therefore, using Equation (7.2.18) of Lemma 7.2.14, we have

$$t(G) \geq \frac{1}{\Delta} \geq \frac{1}{\mu_n - \delta} = \frac{\delta}{\mu_n - \delta} \geq \frac{\mu_2}{\mu_n - \delta}, \tag{7.2.23}$$

confirming the conjecture for graphs with at least one leaf. ∎

Before proceeding, it is worth recalling the following identity we saw in Equation (2.3.2). If L is the Laplacian of a graph G with n vertices, then for any vector $\mathbf{x} \in \mathbb{R}^n$, we have

$$x^T L x = \sum_{\{i,j\} \in E} (x_i - x_j)^2. \tag{7.2.24}$$

Lemma 7.2.20 (Mohar [59])**.** *Suppose X and Y are disjoint vertex subsets of $V(G)$ with no edges between X and Y. Let the number of edges between X and S be a, and the number of edges between Y and S be b, where $S = V \backslash \{X \cup Y\}$. Let $s = |S|, x = |X|$ and $y = |Y|$. Then*

$$\frac{\mu_2}{n} \leq \frac{a+b}{s(x+y)} \leq \frac{\mu_n}{n}. \tag{7.2.25}$$

Using a similar technique, one can deduce the following.

Lemma 7.2.21. *Let G be a graph. Suppose X and Y are disjoint vertex subsets of $V(G)$ with no edges between X and Y. Let $S = V \backslash \{X \cup Y\}$ and $s = |S|, x = |X|$ and $y = |Y|$. Let the number of edges between X and S be a, and the number of edges between Y and S be b. Then*

$$\frac{\mu_2}{n} \leq \frac{a}{x(s+y)} \leq \frac{\mu_n}{n}, \tag{7.2.26}$$

$$\frac{\mu_2}{n} \leq \frac{b}{y(x+s)} \leq \frac{\mu_n}{n}. \tag{7.2.27}$$

Lemma 7.2.22. *Suppose X and Y are disjoint vertex subsets of $V(G)$ with no edges between X and Y and $S = V \backslash \{X \cup Y\}$. Let $s = |S|, x = |X|$ and $y = |Y|$ with $x \leq y$. Then,*

$$s \geq n \frac{\mu_2}{\mu_n} \frac{x}{y}. \tag{7.2.28}$$

Proof: We define a vector $\mathbf{v}$ to be y on the vertices of X, and $-x$ on the vertices of Y, and 0 on the vertices of S. If there are a edges between X and S, and b edges between Y and S then we have the following.

$$\frac{\mathbf{v}^T L\mathbf{v}}{\mathbf{v}^T\mathbf{v}} = \frac{ay^2+bx^2}{xy^2+yx^2} \leq \frac{(a+b)y^2}{xy^2+yx^2}, \text{ since } x \leq y. \tag{7.2.29}$$

Now, from Lemma 7.2.20, we have $a+b \leq \frac{\mu_n}{n}s(x+y)$. Hence we have

$$\frac{\mathbf{v}^T L\mathbf{v}}{\mathbf{v}^T\mathbf{v}} \leq \frac{(a+b)y^2}{xy^2+yx^2} \leq \frac{\frac{\mu_n}{n}s(x+y)y^2}{xy(x+y)} = s\frac{\mu_n}{n}\frac{y}{x}. \tag{7.2.30}$$

Since $\mathbf{v}$ is orthogonal to the $\mathbf{1}$ vector, Corollary 2.3.4 gives

$$\mu_2 \leq \frac{\mathbf{v}^T L\mathbf{v}}{\mathbf{v}^T\mathbf{v}} \leq s\frac{\mu_n}{n}\frac{y}{x},$$

from which we get

$$s \geq n\frac{\mu_2}{\mu_n}\frac{x}{y}$$

as desired. ∎

Remark 7.2.23. Lemma 7.2.22 is not in an easily usable form. It is clear though that if $x=y$, then $s \geq n\frac{\mu_2}{\mu_n}$.

Proposition 7.2.24. *If the vertex connectivity κ of graph G satisfies $\kappa \geq n\frac{\mu_2}{\mu_n}$ then the toughness of G satisfies*

$$t(G) \geq \frac{\mu_2}{\mu_n-\delta}.$$

Proof: For any disconnecting set S, we have $s \geq \kappa \geq n\frac{\mu_2}{\mu_n}$, which together with Equation (7.2.7) gives the desired bound. ∎

Consider the scenario where the size of a disconnecting set S of the graph is less than $n\frac{\mu_2}{\mu_n}$. We conjecture that $c(G-S)$ is at most $\mu_n-\delta$. To validate this conjecture, we verify its accuracy across various graphs, including those obtained through computer searches for graphs with at most 8 vertices.
By using the properties $s \geq \mu_2$ and $c \leq \mu_n - \delta$, we deduce that $t \geq \frac{\mu_2}{\mu_n-\delta}$. This, combined with Proposition 7.2.24, allows us to resolve Conjecture 7.2.2.

Conjecture 7.2.25. Let G be a graph with minimum degree δ, largest Laplacian eigenvalue μ_n and μ_2 as the algebraic connectivity. Let S be a disconnecting set of G. If $|S| < n\frac{\mu_2}{\mu_n}$, then the number of components c of $G - S$ satisfies $c \leq \mu_n - \delta$.

Remark 7.2.26. By computer search, Conjecture 7.2.25 is true for all graphs on at most 8 vertices. Thus, combining this with Proposition 7.2.24, we have the following.

Corollary 7.2.27. *Conjecture 7.2.2 is true for a graph on at most 8 vertices.*

7.2.2 Another Look at Haemers' Toughness Conjecture

In what follows, we show that the conjecture is true, else the bound in Equation (7.2.9) is strict. Thus equality in (7.2.9) implies conjecture being satisfied.

We shall use the following definitions and notations for this section. Let S, X, Y be disjoint vertex subsets of $V(G)$, with no edges between X and Y. For notation, recall $E(A, B)$ is the collection of edges with one endpoint in A and one endpoint in B. Let $s = |S|, x = |X|$ and $y = |Y|$, and suppose $x \leq y$. Define the following edge densities:

$$\alpha = \frac{|E(X,S)|}{xs} = \frac{a}{xs}$$
$$\beta = \frac{|E(Y,S)|}{ys} = \frac{b}{ys}.$$

Lemma 7.2.28. *With the variables as defined, we have the following.*

$$\frac{\mu_2}{s} \leq \frac{y}{x+y}\alpha + \frac{x}{x+y}\beta. \tag{7.2.31}$$
$$\frac{\mu_n}{n} \geq \frac{x}{x+y}\alpha + \frac{y}{x+y}\beta. \tag{7.2.32}$$

Proof: Define $\mathbf{u}$ and $\mathbf{v}$ by:

$$u_j = \begin{cases} y & j \in X \\ -x & j \in Y \\ 0 & j \in S \end{cases}$$
$$v_j = \begin{cases} -s & j \in X \\ -s & j \in Y \\ x+y & j \in S. \end{cases}$$

Observe that $\mathbf{u}$ and $\mathbf{v}$ are orthogonal to the $\mathbf{1}$ vector, thus Rayleigh quotient, Corollary 2.3.4, gives the following:

$$\mu_2 \leq \frac{\mathbf{u}^T L\mathbf{u}}{\mathbf{u}^T\mathbf{u}} = \frac{y^2a + x^2b}{xy^2 + yx^2} = \frac{y^2a}{xy(x+y)} + \frac{x^2b}{xy(x+y)},$$

which leads to

$$\frac{\mu_2}{s} \leq \frac{y}{x+y}\frac{a}{xs} + \frac{x}{x+y}\frac{b}{ys} = \frac{y}{x+y}\alpha + \frac{x}{x+y}\beta.$$

That is,

$$\frac{\mu_2}{s} \leq \frac{y}{x+y}\alpha + \frac{x}{x+y}\beta. \tag{7.2.33}$$

Similarly;

$$\begin{aligned}\mu_n \geq \frac{\mathbf{v}^T L\mathbf{v}}{\mathbf{v}^T\mathbf{v}} &= \frac{(x+y+s)^2a + (x+y+s)^2b}{xs^2 + ys^2 + s(x+y)^2} \\ &= \frac{(x+y+s)^2(a+b)}{s(x+y)(s+x+y)} \\ &= \frac{n}{s(x+y)}\big(a+b\big).\end{aligned}$$

So we have

$$\frac{\mu_n}{n} \geq \frac{1}{x+y}\left[\frac{xa}{xs} + \frac{yb}{ys}\right] = \frac{1}{x+y}(x\alpha + y\beta) = \frac{x}{x+y}\alpha + \frac{y}{x+y}\beta.$$

That is,

$$\frac{\mu_n}{n} \geq \frac{x}{x+y}\alpha + \frac{y}{x+y}\beta. \tag{7.2.34}$$

∎

Now let us explore what happens if Haemers' toughness bound is false. With the variables as defined at the beginning of this section, we have the following.

Proposition 7.2.29. *If Haemers' toughness conjecture (Conjecture 7.2.2) is false then the following are true.*

i. The inequality in bound (7.2.9) *is strict. That is,*

$$t(G) > \frac{\mu_n\mu_2}{n(\mu_n - \delta)}.$$

ii. The toughness of G satisfies

$$t(G) > \frac{\bar{d}}{\mu_n - \delta}$$

where $\bar{d}$ is the average out-degree of vertex set Y, that is, $\bar{d} = \frac{b}{y}$.

Proof: We consider the following two cases;

Case A. If $\alpha \leq \beta$. Then using Lemma 7.2.28 we have

$$\frac{\mu_2}{s} \leq \frac{1}{x+y}(y\alpha + x\beta) \leq \frac{1}{x+y}(x\alpha + y\beta) \leq \frac{\mu_n}{n}.$$

Rearranging gives $s \geq \mu_2 \frac{n}{\mu_n}$. Now, picking a vertex from each of the c components of $G - S$, we have an independent set. Using Theorem 7.2.5 we have $c \leq \frac{\mu_n - \delta}{\mu_n} n$. Thus the toughness satisfies the following.

$$t(G) = \frac{s}{c} > \frac{\mu_2 \frac{n}{\mu_n}}{(\mu_n - \delta)\frac{n}{\mu_n}} = \frac{\mu_2}{\mu_n - \delta},$$

confirming the conjecture for G.

Case B. If $\alpha > \beta$. Then

i. from Equation (7.2.31), we have

$$\frac{\mu_2}{s} \leq \frac{1}{x+y}(y\alpha + x\beta) < \frac{1}{x+y}(y\alpha + x\alpha) = \alpha.$$

Thus, we have $s > \frac{1}{\alpha}\mu_2 \geq \mu_2$ since $\alpha \leq 1$. Therefore, the toughness t satisfies

$$t(G) = \frac{s}{c} > \frac{\frac{1}{\alpha}\mu_2}{\frac{\mu_n - \delta}{\mu_n} n} \geq \frac{\mu_n \mu_2}{n(\mu_n - \delta)},$$

improving and showing the bound given in Equation (7.2.9) is a strict inequality.

ii. we have

$$\frac{b}{ys} = \beta = \frac{1}{x+y}(x\beta + y\beta) < \frac{1}{x+y}(x\alpha + y\beta) \leq \frac{\mu_n}{n}.$$

Thus,

$$s > \frac{b}{y}\frac{n}{\mu_n} = \bar{d}\frac{n}{\mu_n}.$$

Therefore, the toughness t satisfies

$$t(G) = \frac{s}{c} > \frac{\bar{d}\frac{n}{\mu_n}}{\frac{\mu_n-\delta}{\mu_n}n} = \frac{\bar{d}}{\mu_n - \delta},$$

as required.

∎

7.2.3 Haemers' Toughness Conjecture and an Infinite Family of Graphs

In this section we define an infinite family of graphs and confirm Conjecture 7.2.2 for these graphs.

A *clique* K_l is a subset of l vertices in a graph such that every pair of vertices in the subset is connected by an edge. Let $c \geq 2$. We define the graph $J(s, c, \ell)$ as follows: Let S be an independent set of s vertices. Form ℓ disjoint cliques K_s, each connecting every vertex in K_s to a distinct vertex in S to form a matching. Also include $c - \ell$ isolated vertices (K_1), each adjacent to every vertex in S. $J(s, c, \ell)$ thus has $n = s + s\ell + c - \ell$ vertices. Observe that, if $s = 1$, we have a star, which is a graph where one vertex (the center) is adjacent to all other vertices (the leaves), see Proposition 7.2.18. Thus, we can exclude $J(1, c, \ell)$ for the purposes of this section. An illustration of $J(3, 5, 2)$ is given in Figure 7.1.

It is clear from this definition that S is a disconnecting set of $J(s, c, \ell)$ and there are c connected components of $V(J) - S$.

Lemma 7.2.30. *Graph $J(s, c, \ell)$ as defined above has its largest Laplacian eigenvalue bounded by*

$$\mu_n \geq \frac{1}{2}\left[c + (s+1) + \sqrt{[c + (s-1)]^2 - 4\ell(s-1)}\right].$$

Proof: Define $\mathbf{u}$ by:

$$u_j = \begin{cases} 1 & j \in S \\ x & j \in K_1 \\ y & j \in K_s, \end{cases}$$

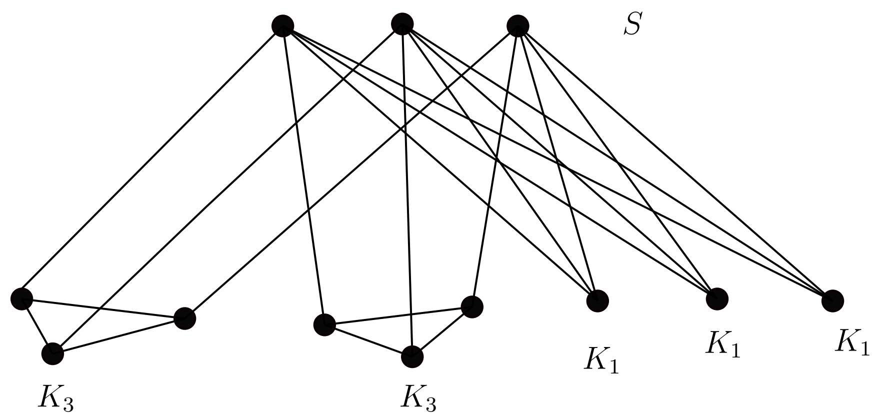

Figure 7.1: Graph $J(3,5,2)$

where

$$y = \frac{x}{s - sx + x}$$

and

$$x = \frac{s}{2(c-\ell)(s-1)}\left[c - (s-1) - \sqrt{[c+(s-1)]^2 - 4\ell(s-1)}\right].$$

Observe that $\mathbf{u}$ is orthogonal to the $\mathbf{1}$ vector, that is, $s + \ell(sy) + (c-\ell)x = 0$ (indeed, the value for x was obtained by solving this relation).

Now recall from Proposition 2.2.4, we have $L\mathbf{u} = \mu\mathbf{u}$ if and only if $\sum_{j\sim i} u_j = (deg(i) - \mu)u_i$ for all i.

Let i be a vertex in S, then

$$\ell y + (c-\ell)x = (c-\mu)1$$
$$\ell\frac{x}{s-sx+x} + cx - \ell x = c - \mu.$$

Thus

$$\mu = c - \frac{[cs - \ell(s-1)]\,x - (c-\ell)(s-1)x^2}{s-(s-1)x}. \qquad (7.2.35)$$

Substituting x into Equation (7.2.35) and tediously simplifying, we obtain

$$\mu = \frac{1}{2}\left[c + (s+1) + \sqrt{[c+(s-1)]^2 - 4\ell(s-1)}\right], \qquad (7.2.36)$$

and thus the required bound.

Similarly, let i be a vertex in K_s, then

$$1 + y(s-1)x = (s-\mu)y$$

$$\mu = 1 - \frac{1}{y} = s - \frac{s}{x}. \tag{7.2.37}$$

Finally, if we let i be a vertex in K_1, then $1s = (s-\mu)x$ so that we get $\mu = s - \frac{s}{x}$, as in Equation (7.2.37).

Now substituting x into Equation (7.2.37) and simplifying, we again obtain (7.2.36), and thus the desired bound. ∎

Lemma 7.2.31. *The graph $J(s,c,\ell)$, as defined above, has its second smallest Laplacian eigenvalue bounded by*

$$\mu_2 \leq \begin{cases} \frac{1}{2}\left[c + (s+1) - \sqrt{[c+(s-1)]^2 - 4(s-1)}\right] & \textit{if } \ell = 1 \\ 1 & \textit{if } \ell \geq 2. \end{cases}$$

Proof: Choosing same vector $\mathbf{u}$ as in the proof of Lemma 7.2.30 and letting x be defined as

$$x = \frac{s}{2(c-\ell)(s-1)}\left[c - (s-1) + \sqrt{[c+(s-1)]^2 - 4\ell(s-1)}\right],$$

and going through the same process in that proof, in particular, substituting x into Equation (7.2.35) and simplifying, we deduce

$$\mu_2 \leq \frac{1}{2}\left[c + (s+1) - \sqrt{[c+(s-1)]^2 - 4\ell(s-1)}\right].$$

But we can do better when $\ell \geq 2$. Let $\mathbf{v}$ be defined as follows: consider any two of the ℓ K_s cliques in the graph $J(s,c,\ell)$. Assign -1 to every vertex in one of these cliques and 1 to every vertex in the other. Set all other vertices in J to 0.

It is evident that $\mathbf{v}$ is orthogonal to the $\mathbf{1}$ vector. Furthermore, 1 is a corresponding eigenvalue of $\mathbf{v}$. Consequently, 1 serves as an upper bound for μ_2, the second smallest eigenvalue of the graph $J(s,c,\ell)$, for $\ell \geq 2$. ∎

Theorem 7.2.32. *The toughness of graph $J(s,c,\ell)$ satisfies*

$$t(J) = \frac{s}{c} \geq \frac{\mu_2}{\mu_n - \delta}.$$

Before we prove Theorem 7.2.32, let us prove a couple of claims.

Claim 1. For $c \geq 2$, $\ell \geq 1$ and $s \geq 2$ where $c, \ell, s \in \mathbf{N}$,

$$c \geq \frac{s}{2}\left[-(s-1)+\sqrt{(s-1)^2+4\ell}\right]. \tag{7.2.38}$$

Proof. [of Claim 1] We simplify Inequality (7.2.38):

$$\begin{aligned} 2c &\geq s\left[-(s-1)+\sqrt{(s-1)^2+4\ell}\right] \\ 2c+s(s-1) &\geq s\sqrt{(s-1)^2+4\ell} \\ (2c+s(s-1))^2 &\geq s^2\left((s-1)^2+4\ell\right) \\ 4c^2+4cs(s-1)+s^2(s-1)^2 &\geq s^2(s-1)^2+4s^2\ell \\ (c-\ell)s^2-cs+c^2 &\geq 0 \end{aligned}$$

Now equation $(c-\ell)s^2-cs+c^2=0$ has roots $s=\dfrac{c \pm c\sqrt{1-4(c-\ell)}}{2(c-\ell)}$ which are complex since $c>\ell$. Thus the inequality $(c-\ell)s^2-cs+c^2 \geq 0$ is always true and thus Inequality (7.2.38) holds.

Claim 2. For $c \geq 2$, $\ell \geq 1$ and $s \geq 2$ where $c, \ell, s \in \mathbf{N}$,

$$\frac{1}{2}\left[c+(s+1)+\sqrt{[c+(s-1)]^2-4\ell(s-1)}\right] \geq \frac{c\mu_2}{s}+s.$$

Proof. [of Claim 2]

$$\begin{aligned} \frac{1}{2}\left[c+(s+1)+\sqrt{[c+(s-1)]^2-4\ell(s-1)}\right] &\geq \frac{c\mu_2}{s}+s \\ c+(s+1)+\sqrt{[c+(s-1)]^2-4\ell(s-1)} &\geq \frac{2c\mu_2}{s}+2s \\ \sqrt{[c+(s-1)]^2-4\ell(s-1)} &\geq \frac{2c\mu_2}{s}+s-c-1 \\ s\sqrt{[c+(s-1)]^2-4\ell(s-1)} &\geq 2c\mu_2+s^2-sc-s \\ s^2\left[c+(s-1)\right]^2-4\ell(s-1) &\geq (2c\mu_2+s^2-sc-s)^2 \\ 4\left[\mu_2(s-\mu_2)c^2+s(s-1)(s-\mu_2)c+\ell s^2(1-s)\right] &\geq 0 \end{aligned} \tag{7.2.39}$$

We consider two cases.

1. If $\ell \geq 2$. Recall from Lemma 7.2.31 that we have $\mu_2 \leq 1$, thus Equation (7.2.39) becomes

$$(s-1)c^2 + s(s-1)^2 c + \ell s^2(1-s) \geq 0 \tag{7.2.40}$$

For $s \neq 1$, the equation

$$(s-1)c^2 + s(s-1)^2 c + \ell s^2(1-s) = 0$$

has roots

$$c = -\frac{s}{2}\left(s - 1 \pm \sqrt{(s-1)^2 + 4\ell}\right).$$

Hence from the inequality (7.2.40) we need to show that

$$c \geq \frac{s}{2}\left(-(s-1) + \sqrt{(s-1)^2 + 4\ell}\right),$$

but this is true by Claim 1.

2. If $\ell = 1$. Then from Inequality (7.2.39), we want to show

$$-c^2\mu_2^2 + cs(c-s+1)\mu_2 + s^2(s-1)(c-1) \geq 0. \tag{7.2.41}$$

But the equation $-c^2\mu_2^2 + cs(c-s+1)\mu_2 + s^2(s-1)(c-1) = 0$ has roots

$$\mu_2 = \frac{s}{2c}\left[c - s + 1 \pm \sqrt{(c-s+1)^2 + 4(s-1)(c-1)}\right].$$

Hence from Inequality (7.2.41), it suffices to show

$$\mu_2 \leq \frac{s}{2c}\left[c - s + 1 + \sqrt{(c-s+1)^2 + 4(s-1)(c-1)}\right].$$

Thus using Lemma 7.2.31, we are done, if we show

$$\begin{aligned} &\frac{1}{2}\left[c + (s+1) - \sqrt{[c + (s-1)]^2 - 4(s-1)}\right] \\ &\leq \frac{s}{2c}\left[c - s + 1 + \sqrt{(c-s+1)^2 + 4(s-1)(c-1)}\right], \\ &\iff c^2 + c - c\sqrt{[c + (s-1)]^2 - 4(s-1)} \\ &\leq -s^2 + s + s\sqrt{(c-s+1)^2 + 4(s-1)(c-1)}. \end{aligned} \tag{7.2.42}$$

Let $f(c,s) = c^2 + c - c\sqrt{[c+(s-1)]^2 - 4(s-1)}$ and $g(c,s) = -s^2 + s + s\sqrt{(c-s+1)^2 + 4(s-1)(c-1)}$. For any c fixed and $c \geq 2$, observe that

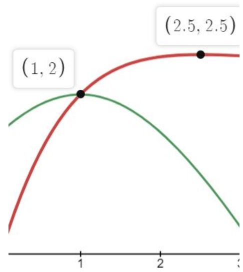

Figure 7.2: $f(c, s)$ (green curve) verse $g(c, s)$ (red curve) when $c = 2$

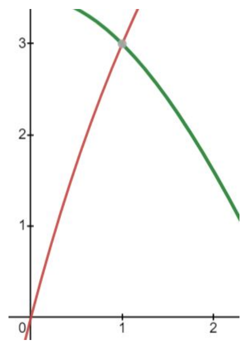

Figure 7.3: $f(c, s)$ (green curve) verse $g(c, s)$ (red curve) when $c \geq 3$

$f(c, 1) = g(c, 1)$. That is, the two functions intercept only at $s = 1$. We also have that

$$f_s(c, s) = \frac{\partial f(c, s)}{\partial s} = -\frac{c(s + c - 3)}{\sqrt{[c + (s - 1)]^2 - 4(s - 1)}}$$

and

$$g_s(c, s) = \frac{\partial g(c, s)}{\partial s} = -2s + 1 + \frac{2s^2 + 3cs - 9s + c^2 - 2c + 5}{\sqrt{(c - s + 1)^2 + 4(s - 1)(c - 1)}}.$$

Now at $c = 2$, we have $f_s(c, s) \leq 0$ for $s > 1$ while $g_s(c, s) \leq 0$ for $s \geq 2.5$. Now since the only intersection of the two functions occur at $s = 1$, we deduce $g(c, s) \geq f(c, s)$ at $c = 2$. See Figure 7.2.

Finally, for $c \geq 3$, we have $f_s(c, s) \leq 0$ for $s \geq 1$ while $g_s(c, s) > 0$ for all s. Since $f(c, 1) = g(c, 1)$, we have that $g(c, s) \geq f(c, s)$ for $c \geq 3$. See Figure 7.3. Hence we have shown that Inequality 7.2.42 is true, which implies Inequality 7.2.41 is true, confirming the claim for $\ell = 1$.

Proof: (**Proof of 7.2.32**)
Observe that $J(s, c, \ell)$ has minimum degree $\delta = s$, thus, it suffices to show $\mu_n \geq$

$\frac{c\mu_2}{s} + s$. Recall from Claim 2 we have

$$\frac{1}{2}\left[c + (s+1) + \sqrt{[c + (s-1)]^2 - 4\ell(s-1)}\right] \geq \frac{c\mu_2}{s} + s,$$

which together with Lemma 7.2.30 gives the desired proof.

∎

7.2.4 Applications

As we mentioned in our introduction, the concept of graph toughness finds application in various contexts. In this section, we delve into some of these applications, particularly focusing on scenarios where the conjectured bound (Conjecture 7.2.2) holds.

r-tough graphs

The condition for a graph to be r-tough is that $t(G) \geq r$. Liu and Chen [52] showed that if $\mu_n - \mu_2 \leq \frac{\mu_2}{2}$, then G is 2-tough. This was generalized by Gu and Haemers [38] as follows; if $\mu_n - \mu_2 \leq \frac{\mu_2}{r}$, then G is r-tough. Whenever Conjecture 7.2.2 is true, we have have the following improvement.

Theorem 7.2.33. *Conjecture 7.2.2 implies if $\mu_n - \delta \leq \frac{\mu_2}{r}$, then G is r-tough.*

Elementary graph property

A graph G is said to be *elementary* if it contains a perfect matching and the edges that occur in a perfect matching in G induce a connected subgraph. In other words, if we take any perfect matching in G, the edges in that matching induce a connected subgraph. An elementary graph is a special type of graph that has a perfect matching and this property is useful in the study of matchings and related topics in graph theory.

Bauer, Broersma, Kahl, Morgana, Schmeichel and Surowiec proved in [8] that any graph with an even number of vertices and 1-toughness property is elementary. Gu and Haemers [38] gave a Laplacian condition for this as follows. If n is even and $\mu_n - \mu_2 \leq \mu_2$, then G is elementary. Thus Conjecture 7.2.2 provides a stronger criterion for determining when a graph is elementary.

Theorem 7.2.34. *Let G be a graph on n vertices where n is even. Then Conjecture 7.2.2 implies if $\mu_n - \delta \leq \mu_2$, then G is elementary.*

k-factor

A *k-factor* of a graph is a k-regular spanning subgraph. For example, a 1-factor of a graph is a perfect matching, and a 2-factor is a collection of edge-disjoint spanning cycles. A k-factor is said to be maximum if it has the largest possible number of edges among all k-factors of the graph.

Enomoto, Jackson, Katerinis, and Saito [26] proved that any k-tough graph G has a k-factor if kn is even and $n \geq k+1$, which confirms Chvátal's conjecture. Katerinis [47] extended this result to non-regular factors. An *$[a,b]$-factor* of a graph G is a spanning subgraph H such that $a \leq deg(H)(v) \leq b$ for each vertex v in G. Katerinis showed that if a graph G on n vertices satisfies $a < b$ or bn is even, and if $t(G) \geq a + \frac{a}{b} - 1$, then G has an $[a,b]$-factor. Conjecture 7.2.2 improves the result by Gu and Haemers [38].

Theorem 7.2.35. *Let $a \leq b$ be positive integers such that $a < b$ or bn is even. Then Conjecture 7.2.2 implies if*

$$\frac{\mu_2}{\mu_n - \delta} \geq a + \frac{a}{b} - 1, \tag{7.2.43}$$

then G has a $[a,b]$-factor.

Let $b > 2$ and G has $n \geq 3$ vertices. Chen [18] showed G has $[2,b]$-factor if $t(G) \geq 1 + \frac{1}{b}$. Whenever Conjecture 7.2.2 holds, we obtain the following result.

Theorem 7.2.36. *Let $b > 2$ and $n \geq 3$. Conjecture 7.2.2 implies if*

$$\mu_n - \delta \leq \frac{b\mu_2}{b+1}, \tag{7.2.44}$$

then G has $[2,b]$-factor.

Conjecture 7.2.2 also improves the generalization given by Gu and Haemers [38] on the Laplacian condition of k-factors by Brouwer and Haemers [13].

Theorem 7.2.37. *Let k be a positive integer such that $n \geq k+1$ and kn is even. Conjecture 7.2.2 implies if*

$$\mu_n - \delta \leq \frac{\mu_2}{k}, \tag{7.2.45}$$

then G has a k-factor.

A graph G is called *factor-critical* [53] if $G - v$ has a perfect matching, for all $v \in V(G)$. It was shown in [8] that a 1-tough graph on an odd number of vertices is factor-critical. Generally, a graph G is said to be *(k,ℓ)-factor-critical* if $G - X$ has a k-factor for all $X \subset V(G)$ with $|X| = \ell$. A $(1,1)$-factor-critical graph is commonly known as factor-critical graph. In [38], it was given that, if n is odd and $2\mu_2 \geq \mu_n$, then G is $(1,1)$-factor-critical. Conjecture 7.2.2 would improve this result.

Theorem 7.2.38. *Conjecture 7.2.2 implies if n is odd and $\mu_n - \delta \le \mu_2$, then G is $(1,1)$-factor-critical.*

Favaron [27] showed that if a graph G has n vertices with $2 \le s < n$, and $n+s$ is even, then if $t(G) > \frac{s}{2}$, then G is a $(1,s)$-factor-critical graph. Conjecture 7.2.2 would lead to the following result.

Theorem 7.2.39. *Suppose $2 \le s < n$ and $n+s$ is even. Conjecture 7.2.2 implies if*

$$\mu_n - \delta \le \frac{2\mu_2}{s}, \tag{7.2.46}$$

then G is a $(1,s)$-factor-critical.

Spanning trees

A theorem of Win [68] implies G has a spanning tree with maximum degree at most k if $t(G) \ge \frac{1}{k-2}$ for $k \ge 3$.

Theorem 7.2.40. *Let $k \ge 3$ be an integer. Conjecture 7.2.2 implies if*

$$\mu_n - \delta \le (k-2)\mu_2,$$

then G has a spanning tree with maximum degree at most k.

A k-walk in a graph G is a closed spanning walk of G that visits every vertex of G at most k times. This generalizes the idea of Hamiltonian cycles in G. Ellingham and Zha [25] showed that every 4-tough graph has a 2-walk. Whenever Conjecture 7.2.2 holds, we obtain a Laplacian eigenvalue condition for the existence of a 2-walk.

Theorem 7.2.41. *Conjecture 7.2.2 implies if $\mu_n - \delta \le \frac{\mu_2}{4}$, then G has a 2-walk.*

m-extendable graphs

Suppose we have a graph G with n vertices and a perfect matching, and let m be a positive integer such that m is less than $n/2-1$. A graph G is called m-extendable if for every matching M of size m in G, there exists a perfect matching in G containing M. In particular, every matching of size m can be extended to a perfect matching. Plummer proved in [61] that every m-extendable graph is r-tough for $r \ge m$. Conjecture 7.2.2 would give the following.

Theorem 7.2.42. *Suppose n is even, and let m be a positive integer such that $m < n/2-1$. Conjecture 7.2.2 implies if*

$$\mu_n - \delta \le \frac{\mu_2}{m},$$

then G is an m-extendable graph.

Chapter 8

Concluding Remarks

In this thesis, we systematically applied tools of quotient matrices and eigenvalue interlacing to explore fundamental graph parameters, focusing on independence, connectivity, and toughness.

Regarding the k-independence of graphs, we built upon the work of Abiad et al. [1, 2] who extended Hoffman's spectral bounds to k-independence. While optimal polynomials for $k = 1$ and $k = 2$ had already been identified by these researchers, our contribution lies in determining the optimal polynomial for $k = 3$. We applied this polynomial to various graph families, including the Johnson graphs, Odd graphs and Hamming graphs, establishing bounds that proved to be tight in several instances. For instance, we demonstrated the tightness of the bound for the Hamming graph $H(d, 2)$, also known as the hypercube, by constructing 3-independent sets in $H(d, 2)$. This has implications for coding theory, as codes and anticodes are k-independent sets in the Hamming graph. A set of codewords that satisfy an upper bound on their pairwise Hamming distance is called anticode.

Our investigation uncovered a common pattern in optimal polynomials for $k = 1, 2, 3$, which suggests that, in general, an optimal polynomial $p(x)$ has $\lambda(p)$ at k distinct eigenvalues, occurring for some index set $I \subset \{1, \ldots, d\}$ of size $|I| = k$ and $d \in I$ if k is odd. That is, $\lambda(p) = \prod_{i \in I} \theta_i = p(\theta_i)$ for $i \in I$.

Alternatively, an optimal polynomial is of the form $f(x) = \prod_{i \in I}(x - \theta_i)$ where $\lambda(f) = f(\theta_i) = 0$ for all $i \in I$. This is consistent with Fiol's minor polynomials, which serve as a normalization of $f(x)$. The primary challenge lies in selecting the appropriate indices, representing the eigenvalues of the graph. We noted that these indices must come in consecutive pairs, that is, the condition on the index set I is that $i_{2j} = i_{2j-1} + 1$ for $j = 1, 2, 3, \ldots, \lfloor \frac{k}{2} \rfloor$. Resolving this index selection challenge would complete the polynomial method for bounding the k-independence number.

The ongoing challenge of identifying suitable indices that represent the eigenvalues of the graph, especially for higher values of k, coupled with the complexity of determining the number of walks on the vertices of the graph, prompts us to introduce certain assumptions or restrictions on the graphs. By assuming that the graphs possess a girth greater than k, we can focus our exploration of closed walks on the vertices of graphs that exhibit local characteristics akin to regular trees. Generating functions for these walks have been determined [58, 63]. We use a combinatorial approach, utilizing the Catalan and Borel triangles. We expressed the number of closed walks in terms of these two number arrays. The result shows that the number of closed walks centered on a vertex forms a polynomial in d, the degree of the graph, with coefficients aligning with the elements of the Borel triangles. This introduces another combinatorial object where the Borel triangle and the Catalan triangle play a crucial role.

In the domains of connectivity and toughness, we presented an improved bound on the vertex connectivity of (n, d, λ)-graphs, building upon the initial proposal by Krivelevich and Sudakov. Exploring graph toughness, we derived new bounds on graph toughness, both general and spectral. Though it remains unresolved, we made progress toward the resolution of Haemers' Laplacian toughness conjecture, confirming its validity for several graph classes, including regular bipartite graphs, trees, graphs with at least one leaf, and graphs on at most 8 vertices.

We believe our approach in showing the conjecture holds for graph $J(s, c, \ell)$ in subsection 7.2.3 may be extended to prove the conjecture in general, if one can monitor the changes in μ_2 and μ_n as we add new vertices and edges to the various components of $J(s, c, \ell)$, and we intend to pursue this in future works.

Many graphs seem to have vertex connectivity satisfying $\kappa \geq \mu_2 \frac{n}{\mu_n}$. In this case, combining it with the Laplacian upper bound on the independence number of the graph resolves the conjecture. Some graphs have $c(G - S) \leq \mu_n - \delta$ and this seems to be the case for graphs that have disconnecting sets that satisfy $|S| < \mu_2 \frac{n}{\mu_n}$. Using computer search, we were able to verify this assertion for graphs with up to 8 vertices. Thus, resolving the following conjecture will imply a resolution of Haemers' conjecture.

Conjecture 8.0.1. If S is a disconnecting set of a graph G, then whenever $|S| < n\frac{\mu_2}{\mu_n}$, the number of components c in $G - S$ is $c \leq \mu_n - \delta$, where δ is the minimum degree of G, μ_n is the largest Laplacian eigenvalue of G, and μ_2 is the algebraic connectivity of G.

Haemer's toughness conjecture could also be resolved by addressing the following conjecture.

Conjecture 8.0.2. Let G be a graph with minimum degree δ. Let $S \subset V$ be such that $G - S$ is disconnected. Let X and Y be disjoint vertex subsets of $V \backslash S$ such that $X \cup Y = V \backslash S$ with $|X| \leq |Y|$. Then

$$|S| \geq \frac{2\mu_2}{\mu_n - \delta}|X|. \tag{8.0.1}$$

Recall that Conjecture 8.0.2 is the hypothesis of Theorem 7.2.12.

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