Spectral Distributions of Sparse Random Graphs and Matrices

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Abstract

B.Sc (Hons)

Spectral Distributions of Sparse Random Graphs and Matrices

by Lukas FESSER

Over the last 30 years, random graphs have become standard tools in both pure and applied mathematics, the most widely-used example being Erdös-Rényi type random graphs [4]. Random graphs are often studied through the eigenvalue distributions of their adjacency matrices, but despite their popularity, little is known about the adjacency spectra of Erdös-Rényi graphs with a very large number of vertices n and a very low probability p of two vertices being connected [16, 17].

This project introduces two approaches to quantify the spectral gap, i.e. the distance between the least negative eigenvalue and the least positive eigenvalue (LPE) of a sparse Erdös-Rényi graph. We show why a partial solution due to Godsil [9] cannot fully solve the problem, before presenting an alternative approach taken by Spiridonov [16]. We prove several of the conjectures made in Spiridonov, improve upon his results, and present several new conjectures that should be useful to fully quantify the spectral gap.

Statement of the Author's Original Contributions

1. The numerical results in section 3.2 are our own, as is the code that generated these results.

2. Theorem 4.1.1 is our original proof of a claim first made in [9], and so is Corollary 4.1.2.1.

3. Theorem 4.1.5 is our original statement and proof of a theorem that is probably well known, but which we could not find in print.

4. Theorem 4.1.3 is our original proof of a claim first made in [9]. Lemma 4.1.4 is an original result (statement and proof).

5. Counterexample 4.1.1 is our own, as is Counterexample 4.2.1.

6. Theorem 4.2.2 is an original result (statement and proof).

7. Theorem 4.2.4 is our original proof of a conjecture first made in [16].

8. The conjectures at the end of section 4.2.1 are our own, based on our earlier numerical results.

9. Theorem 4.2.5 is our original proof of a claim first made in [16]. Theorem 4.2.6 is a partial proof of another claim in [16].

Contents

List of Figures

Chapter 1

Introduction

"As long as a branch of science
offers an abundance of problems,
so long it is alive"

David Hilbert

1.1 Background & Motivation

Random graph theory is a part of mathematics that employs probabilistic methods to establish results in graph theory . In the 1940s, Hungarian mathematician Paul Erdös was the first to use random graphs to give probabilistic constructions of graphs with particular properties, such as large girths and large chromatic numbers [4]. Erdös' 1959 paper "On Random Graphs" with fellow Hungarian mathematician Alfred Rényi began the field now known as random graph theory by systematically studying random graphs as objects of mathematical interest in their own right [7].

Today, random graph theory is a major field of interest in discrete mathematics and theoretical computer science [15]. Within graph theory itself, random graphs can also help us answer questions that ask about a "typical" graph [4]. We might, for example, be interested in the size of the largest clique in a typical graph, or the length of the shortest cycle. Random graphs can help us get estimates for many of these questions.

In addition, random graph theory has also been applied to complex networks in biology, to the internet, and to social networks [4, 11, 12]. Social networks in particular tend to be far too large to examine in detail, which results in the need for approximate models. Based on these models, we may ask questions about the expected number of contacts that each individual in the network has, or how large we expect the largest connected group of individuals to be.

Over the last twenty years, these questions on the structural properties of complex networks and the methods to answer them have become collectively known as Network Science, or Network Theory. As a branch of applied mathematics, Network Science concerns itself with the understanding, mathematical description, prediction, and control of complex systems [15].

It is founded on the observation that behind each complex system - be it a network describing the interactions between genes and proteins in metabolism, the sum of all professional, friendship, and family ties in a society, or the network of generators and transmission lines forming a power grid - behind each of these systems, there is an intricate network that encapsulates the interactions between the system's various components [12, 15].

For the remainder of this paper, we proceed as follows: chapter 2 introduces the definitions and results from graph theory that we will be using and gives an overview of the matrices associated with a graph and the closely related field of spectral graph theory. We conclude chapter 2 with the definition of the Erdös-Rényi model and its connections to more modern random graph models.

Chapter 3 focuses on the spectral distribution of an Erdös-Rényi graph and in particular introduces the notion of sparsity. We present our numerical results on the decay of the spectrum as sparsity increases and elaborate on the role of tree spectra in order to understand the spectrum of a larger graph. In particular, we explain why an understanding of the least positive eigenvalue (LPE) of an arbitrary tree is necessary to quantify the spectral gap of a sparse Erdös-Rényi graph.

In chapter 4, we present two approaches from the literature to determine the LPE of a tree of size k. We show why it is possible to do so for trees of even size, and present several of our own results that should be useful in solving the as yet open case for trees of odd size.

Chapter 2

(Random) Graphs and Matrices

"Graph Theory, more than any other branch of mathematics, feeds on problems"

Béla Bollobás

2.1 Definitions and Prerequisites

2.1.1 Graph Theory

In this section, we provide an overview of the definitions and theorems from graph theory that we will be using throughout this report. We assume a basic familiarity with discrete mathematics at the undergraduate level and focus only on the concepts and results that will be relevant for later chapters. For a more in-depth study of modern graph theory, see [3]. In the following, all graphs are assumed to be simple, i.e. there are no loops joining a vertex to itself, and there can be at most one edge joining two distinct vertices.

Definition 2.1.1. (Subgraph): Let $G = (V, E)$ be a given graph. Then $G' = (V', E')$ is a *subgraph* of G if $V' \subset V$ and $E' \subset E$, which we denote by $G' \subset G$. If G' contains all the edges in G that connect two vertices in V', then G' is called a subgraph spanned or *induced by* V'. We denote this by $G[V']$. G' is called a *spanning subgraph* of G.

Definition 2.1.2. (Walk, Cycle): A *walk* W in a graph is an alternating sequence of edges and vertices, for example $x_0, e_1, x_1, ..., e_n, x_n$, where e_i denotes the edge $x_{i-1}x_i$, $0 < i \leq n$. A walk W for which $x_0 = x_n$, $n \geq 3$, and for which the vertices x_i, $0 < i < n$ are distinct from each other and from x_0 is said to be a *cycle*.

Definition 2.1.3. (Connected Graph, Graph Component): A graph G is said to be *connected* if for every pair of distinct vertices $\{x_0, x_n\}$, there exists a *path*, i.e. a graph P of the form $V(P) = \{x_0, x_1, ..., x_n\}$ and $E(P) = \{x_0x_1, x_1x_2, ..., x_{n-1}x_n\}$,from x_0 to x_n. We call a maximal connected subgraph of G a *component* of G.

Definition 2.1.4. (Tree, Forest): A graph G with no cycles is called a *forest*; a connected forest is called a *tree*.

Definition 2.1.5. (k-partite Graph): We call a graph G *k-partite* with vertex classes $V_1, V_2, ..., V_k$, if $V(G) = V_1 \cup V_2 \cup ... \cup V_k$, $V_i \cap V_j = \emptyset$ whenever $1 \leq i < j \leq k$, and no edge joins two vertices in the same vertex class. We denote a *complete k-partite graph* by $K(n_1, ..., n_k)$.

We now proceed with some elementary results on bipartite graphs and trees in particular. We omit extensive proofs and instead refer the reader to [3] for details.

Theorem 2.1.1. A graph is a forest if and only if for every pair $\{x, y\}$ of distinct vertices, it contains at most one $x - y$ path.

Theorem 2.1.2. Let G be a graph, then the following are equivalent:

1. G is a tree
2. G is a minimal connected graph, i.e. G is connected, but once we remove an edge $xy \in E(G)$, then $G - xy$ is disconnected
3. G is a maximal acyclic graph, i.e. G is acyclic and if x and y are nonadjacent vertices of G, then $G + xy$ contains a cycle.

Theorem 2.1.3. Every connected graph contains a **spanning tree** - a tree containing every vertex of the graph.

Theorem 2.1.4. Let G be a graph of order n. Then the following are equivalent:

1. G is a tree

2. G is connected and has at most $n-1$ edges

3. G is acyclic and has at least $n-1$ edges

4. $G = K_n$ for $n = 1, 2$, and if $n \geq 3$, then $G \neq K_n$ and the addition of an edge to G produces exactly one new cycle.

2.2 Spectral Graph Theory

In the previous section, we recalled some of the basic notions of graphs and trees and gave several results related to these concepts. Graph theory is interesting in and of itself, but in order to study graphs and in particular trees in more detail, we would like to use more tools than the combinatorial techniques we have encountered so far.

In this section, we introduce the matrices related to a graph G - its adjacency matrix $A(G)$, its degree matrix $D(G)$, and its Laplacian $L(G)$ - and briefly discuss the eigenvalues of these matrices and what they tell us about the properties of the graph itself. For a more in-depth study of spectral graph theory, see for example [12, 15].

2.2.1 The Matrices associated with a Graph

Definition 2.2.1. (Adjacency Matrix): Let G be a graph and define a matrix A_G, called the *adjacency matrix* of G, by

$$A_G(i,j) = \begin{cases} 1 \text{ if } (i,j) \in E(G) \\ 0 \text{ otherwise} \end{cases}$$

If G is a graph on n vertices, then A_G is an $n \times n$ matrix. Since we are only considering undirected graphs, A_G is symmetric. Its entries are all real, so A_G is *Hermitian*. We will return to this in the next section.

Definition 2.2.2. (Degree Matrix): For a given graph G, we define its *degree matrix* D_G by

$$D_G(a,b) = \begin{cases} d(a) \text{ if } a = b \\ 0 \text{ otherwise} \end{cases}$$

Note that the degree matrix is thus necessarily a diagonal matrix. Now that we have defined both the adjacency matrix and the degree matrix of a graph G, we may define the Laplacian matrix as well.

Definition 2.2.3. (Laplacian Matrix): Let G be a graph. Then we define its *Laplacian matrix* L_G by $L_G = D_G - A_G$

We will primarily be working with the adjacency and Laplacian matrices of a graph G. We will, however also require a special version of the **incidence matrix** of a graph:

Definition 2.2.4. (Incidence Matrix): Let $G = (V, E)$ be a graph on n vertices and m edges. Then we define its incidence matrix to be the $n \times m$ matrix $B = B(G)$, with

$$B_{ij} = \begin{cases} 1 \text{ if the vertex } v_i \text{ and the edge } e_j \text{ are incident} \\ 0 \text{ otherwise} \end{cases}$$

We care about the eigenvalues of these matrices because of the information on the topology of the graph that they contain. The algebraic multiplicity of the zero eigenvalue of the Laplacian matrix, for example, corresponds to the number of connected components in the graph [15].

2.3 Random Graph Models

In this section, we introduce our primary object of interest: random graphs. We begin with an overview of Erdös-Rényi random graphs, their definition and their properties, as established by Erdös and Rényi around 1960.

For a study of more recent random graph models, in particular Preferential Attachment random graphs and the Small World model, we refer the reader to [11, 13].

2.3.1 The Erdös-Rényi Model

Definition 2.3.1. (Erdös-Rényi Graph): We call a random graph on n vertices and with probability parameter p an Erdös-Rényi graph that is labeled by the elements of $[n]$. Let i and j be two vertices. Then with probability $p = \alpha/n$, we include an edge between these two vertices, independent of other edges. We denote the ensemble of these graphs by $G(n, p)$.

It is worth noting that if we denote the adjacency matrix of G by $A(G)$, then the spectrum of $A(G)$ is now random, since the entries of $A(G)$ are. Hence for random graphs, we speak of the *spectral distribution* of $A(G)$.

The spectral distributions of Erdös-Rényi random graphs will be the main object of study for the remainder of this paper. We devote the entirety of chapter 3 to understanding how the spectrum behaves for different values of p.

Chapter 3

Adjacency Spectra of Sparse Random Graphs

"If I experiment enough, I get a deeper understanding."

Terence Tao

3.1 Continuous and Discrete Spectra

Recall that we construct an Erdös-Rényi, or $G(n, p)$, model by randomly connecting a set of n vertices: each possible edge is included with probability p, independent of all the other edges.

As for the size of p, we distinguish between the following cases:

1. $G(n, p)$, when $p = \omega\left(\frac{1}{n}\right)$ (here, by $f(n) = \omega(g(n))$, we mean that $f(n)/g(n) \to \infty$): in this case, and assuming that $p \leq \frac{1}{2}$, the limiting distribution of the spectrum of the adjacency matrix $A(G)$ is the semicircle distribution first introduced by Wigner in 1955 [17]. Formally,

Theorem 3.1.1. Let $p = \omega\left(\frac{1}{n}\right)$ and assume $p \leq \frac{1}{2}$. For a random graph $G(n, p)$, denote its adjacency matrix by A_n. Then as $n \to \infty$, the empirical spectral distribution (ESD) of the matrix $\frac{1}{\sqrt{np(1-p)}} A_n$ converges in distribution to Wigner's semicircle distribution with density $\rho_{sc}(x)$, supported on the closed interval $[-2, 2]$, where

$$\rho_{sc}(x) = \frac{1}{2\pi}\sqrt{4 - x^2}$$

2. $G(n, p)$, when $p = \frac{\alpha}{n}$: for $p = O\left(\frac{1}{n}\right)$, the ESD of G seems to no longer converge to the semicircle distribution [8, 17]. The spectrum seems to be a composition of a discrete and a continuous part. For small α, the discrete spectrum dominates; for large α, the distribution becomes increasingly determined by the continuous component. As α gets larger, the continuous spectrum seems to approach a semicircle.

The first case is quite well understood [2]. In this paper, we will be focusing on the second case, i.e. we restrict ourselves to sparse random graphs of the form $G(n, \frac{\alpha}{n})$, where $p = \frac{\alpha}{n}$ and $p = O\left(\frac{1}{n}\right)$.

Qualitatively, we can describe the structure of $G(n, p)$ for different p as follows: for small enough p, the graph breaks into various connected components [17]. For $p = \frac{\alpha}{n}$, where α is fixed and $n \to \infty$, Erdös and Rényi [8] describe the following behavior:

- For $\alpha < 1$, all the components of G will be of size $O(\log n)$ almost surely, with most of them being trees.

- For $\alpha = 1$, the largest component of G has a size of the order of $n^{2/3}$ almost surely.
- For $\alpha > 1$, there almost surely exists a largest component (in the following called the giant component of G) of size $g(\alpha)n$, where g is a continuous function, s.t. $g(\frac{1}{2}) = 0$ and $\lim_{\alpha\to\infty} g(\alpha) = 1$. All other components have size $O(\log n)$ as above, with most of them being trees.

3.2 Numerical Results

Our numerical results serve two main goals: first, we illustrate the evolution of the spectrum described in the previous section and reproduce the results in [16] and [17]. We then focus on the first case ($\alpha < 1$) and use numerical tools to gain a better understanding of the adjacency matrices of trees of small size. Our conjectures in section 4.2.1 are based on these results.

Figure 3.1 shows the observed (normalized) eigenvalue distribution for $G(n, \alpha/n)$ when $n = 100$ for various values of α. For a fixed α, we randomly generate 100 graphs on 100 vertices. For each graph, we normalize the adjacency matrix (i.e. we subtract the mean and divide by the standard deviation). We then compute the eigenvalues of the normalized adjacency matrix, collect all 10000 eigenvalues, and plot them as a histogram.

Note that we are primarily interested in the first two rows of Figure 3.1, i.e. in the spectral distributions of $G(n, \alpha/n)$ graphs with low α.

We know that the spectrum of a graph can be formed by combining the spectra of the connected components of the graph [17]. Our idea here is that if the limiting spectrum exists (see [16] for a discussion of this), then we may compute it explicitly by first calculating the spectra of all trees up to the desired size, adding them together, and then normalizing by frequency.

All our numerical results and the MATLAB code used to obtain them are available on a separate GitHub repository. We refer the reader to the appendix for more information on this.

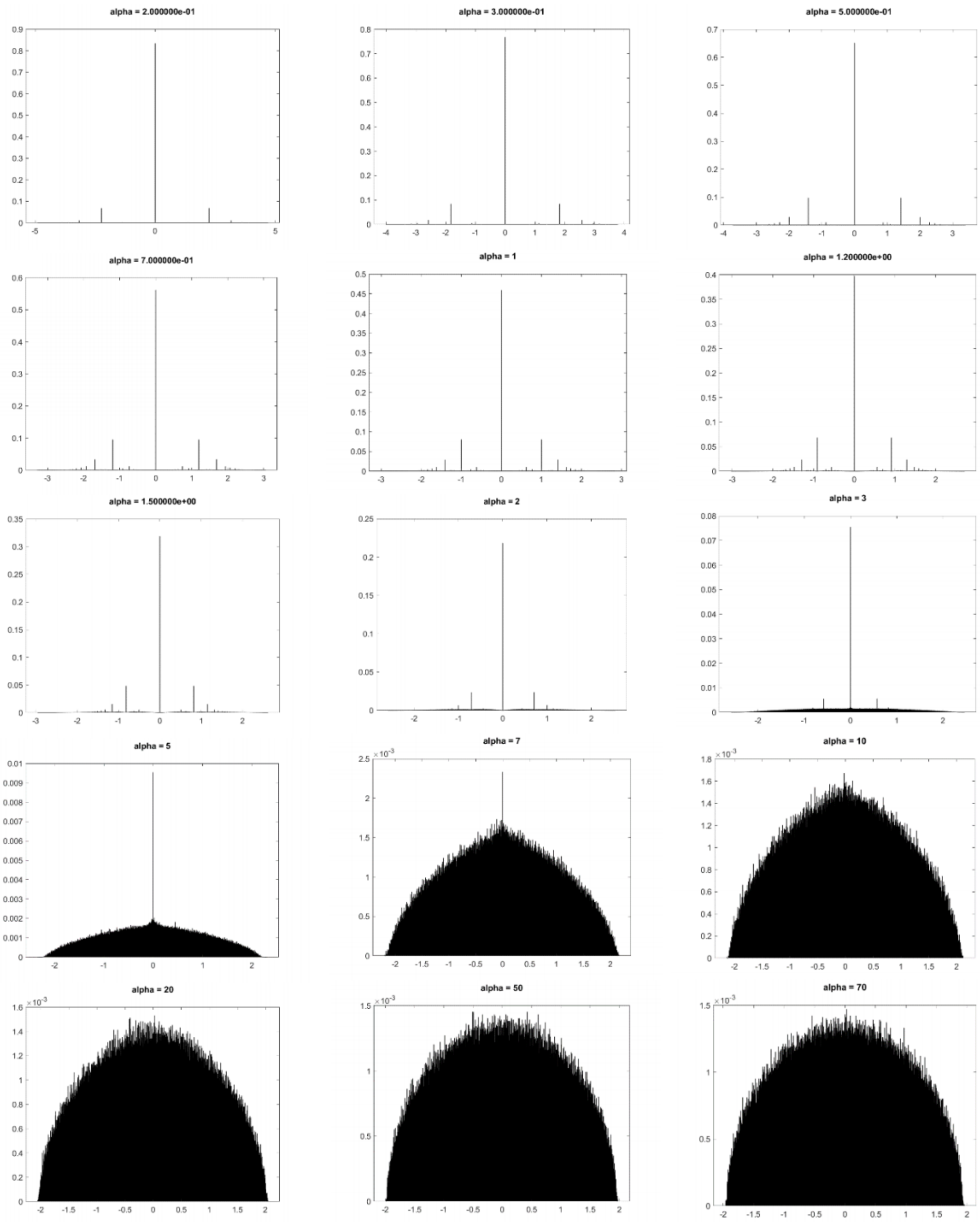

FIGURE 3.1: Normalized empirical spectral distribution of $G(n, \frac{\alpha}{n})$ for various values of α. Taken with $n = 100$ using 100 trials.

Chapter 4

Least Positive Eigenvalues of Trees

In this section, we continue our discussion on adjacency spectra of sparse random graphs. As previously mentioned, we can study the spectrum of the entire graph by studying the spectra of the trees into which it decomposes. In particular, in order to find the LPE of a sparse random graph, and hence characterize its spectral gap, it is sufficient to understand what the LPE of an arbitrary tree is.

Godsil in [9] showed that the LPE of a tree on $2k$ vertices is $2\cos\left(\frac{\pi n}{2n+1}\right)$ using tree inverses. The case for an arbitrary odd tree (i.e. a tree on $2k+1$ vertices) is, to the best of our knowledge, still an open question. We will begin this section by investigating Godsil's proof and show what parts of it can (or cannot) be generalized to odd trees.

In the second half of this section, we will present an alternative approach using characteristic polynomials of adjacency matrices first suggested by Spiridonov [16]. We then present our main results and how they can get us closer to a solution of the problem for odd trees. We conclude with an overview of what we have been able to show in this capstone and give an outline of what future research might look like.

4.1 LPEs through Tree Inverses

We will follow the structure of Godsil's original paper and begin by introducing tree inverses, before showing how they can be applied to solve the LPE problem for trees (or more general bipartite graphs) of size $2k$.

4.1.1 Incidence Matrices and Tree Inverses

Let $G = (V(G), E(G))$ be a bipartite graph. Then by definition, there exists a bipartition (V_1, V_2) of $V(G)$, such that $V(G) = V_1 \cup V_2$ and $V_1 \cap V_2 = \emptyset$. Godsil [9] defines the incidence matrix of G, denoted $B(G)$, as follows

Definition 4.1.1. Let $G = (V, E)$ be a bipartite graph on n vertices. Let (V_1, V_2) be a bipartition of V. Then we define the **Godsil matrix** (also known as the incidence matrix due to Godsil) of G, denoted $B(G)$, by setting $B_{ij} = 1$ if the i-th vertex in V_1 and the j-th vertex in V_2 are adjacent, and $B_{ij} = 0$ if not.

Note that this definition is different from the modern definition of the incidence matrix, which we presented in chapter 2. We shall refer to this new matrix as the Godsil matrix. If $A(G)$ denotes the adjacency matrix of G, then we may represent $A(G)$ by

$$\begin{bmatrix} 0 & B(G) \\ B(G)^T & 0 \end{bmatrix}$$

We have the following result on the invertibility of $A(G)$ and $B(G)$:

Theorem 4.1.1. $A(G)$ is invertible if and only if $B(G)$ is invertible.

Proof: We may assume that $B(G)$ is a square matrix, i.e. that $|V_1| = |V_2|$, otherwise there is nothing to prove. Let $A(G)$ be an $n \times n$ matrix, so that $B(G)$ and $B(G)^T$ are $\frac{n}{2} \times \frac{n}{2}$ matrices.

($\rightarrow$) Let $B(G)$ be invertible. Then $B(G)^T$ is also invertible, so the $\frac{n}{2}$ column vectors of $B(G)$ are linearly independent of each other, and the $\frac{n}{2}$ column vectors of $B(G)^T$ are linearly independent of each other as well. Consider the column vectors of $B(G)$ and append $\frac{n}{2}$ zeros to get the last $\frac{n}{2}$ column vectors of $A(G)$, which are then also linearly independent of each other. Denote these vectors by $u_1, ..., u_{\frac{n}{2}}$. By analogy, the same follows for the first $\frac{n}{2}$ column vectors of $A(G)$, denote these by $v_1, ..., v_{\frac{n}{2}}$.

Suffice it to show that the first $\frac{n}{2}$ column vectors of $A(G)$ are independent of the second $\frac{n}{2}$. Suppose not. Then there exists $v_k \in \{v_1, ..., v_{\frac{n}{2}}\}$, such that

$$v_k = \sum_{i=1}^{\frac{n}{2}} \alpha_i u_i$$

for scalars $\alpha_1, ..., \alpha_{\frac{n}{2}}$. Note that this implies that the last $\frac{n}{2}$ components of $u_1, ..., u_{\frac{n}{2}}$ add up to the $\frac{n}{2}$-dimensional zero vector, which implies that the column vectors of $B(G)^T$ are linearly dependent, so $B(G)^T$ is singular. Contradiction.

The column vectors of $A(G)$ are linearly independent, so $A(G)$ is invertible.

($\leftarrow$) Conversely, suppose $B(G)$ is not invertible. Let $v_1, ..., v_{\frac{n}{2}}$ be the column vectors of $B(G)$. $v_1, ..., v_{\frac{n}{2}}$ is a linearly dependent set, so without loss of generality, we may assume that

$$v_{\frac{n}{2}} = \sum_{i=1}^{\frac{n}{2}-1} \alpha_i v_i$$

for scalars $\alpha_1, ..., \alpha_{\frac{n}{2}}$. As before, append $\frac{n}{2}$ zeros to each vector to get the $\frac{n}{2}$ last column vectors of $A(G)$. Denote these by by $v'_1, ..., v'_{\frac{n}{2}}$. Then we have that

$$v'_{\frac{n}{2}} = \sum_{i=1}^{\frac{n}{2}-1} \alpha_i v'_i$$

for the same scalars $\alpha_1, ..., \alpha_{\frac{n}{2}}$ as before. The column vectors of $A(G)$ are linearly dependent, so $A(G)$ is not invertible.

$\square$

The Godsil matrix $B(G)$ is related to the graph topology of G through the following lemma:

Lemma 4.1.2. Let G be a bipartite graph with bipartition (V_1, V_2). Then G has a unique perfect matching if and only if the vertices in V_1 and V_2 can be ordered so that $B(G)$ is a lower triangular matrix, with all its diagonal entries equal to one.

For a proof, see [9]. We immediately get the following corollary, which we shall from now on use without explicit mention.

Corollary 4.1.2.1. If G is a bipartite graph with a unique perfect matching, then $A(G)$ is invertible.

Proof: By the previous result, it suffices to show that $B(G)$ is invertible. Let G be a bipartite graph with bipartition (V_1, V_2), and let G have a unique perfect matching. Then by Lemma 2.1 in [9], the vertices in V_1 and V_2 can be ordered in such a way that the Godsil matrix $B(G)$ is a lower triangular matrix with all its entries on the main diagonal equal to one. Then $|B(G)| = 1$, so $B(G)$ is invertible.

$\square$

Note that every tree is a bipartite graph. If in addition, G is a tree, then the converse is also true.

Theorem 4.1.3. Let G be a tree whose adjacency matrix $A(G)$ is invertible. Then G has a unique perfect matching.

We require the following lemma:

Lemma 4.1.4. Let G be a tree on n vertices and let i be the multiplicity of the zero eigenvalue in $A(G)$. Then the largest matching in the tree is of size $(n - i)/2$.

Proof: This follows immediately from the result at the end of this section.

□

Proof of 4.1.3: If $A(G)$ is invertible, then we must have that $|G| = 2n$ for some $n \in \mathbb{N}$. The multiplicity of the zero eigenvalue must be 0, so the size of the largest matching in G is $(2n - 0)/2 = n$ by the Lemma, so G has a perfect matching.

Suffice it to show that if a tree has a perfect matching, then that matching has to be unique. Let $T = (V, E)$ be a tree and let M and N be two perfect matchings for T. Consider the graph $G = (V, M \cup N)$ and note that $M \cup N \subset E$. By assumption, M and N cover all vertices, so that every (connected) component of G is either a single edge, and hence included in both M and N, or a cycle. T is a tree, so there can be no cycles, and hence we must have that $M = N$.

□

Theorem 4.1.5. Let G be a tree on n vertices. Then the characteristic polynomial of $A(G)$ has the form

$$\sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} a_i(-1)^{n-i}\lambda^{n-2i}$$

where a_i is the number of matchings of size i and $a_0 = 1$.

Proof: In the following proof, we use Spiridonov's method of recursively computing the characteristic polynomial of a tree (section 5.2.1 in [16]). For the sake of simplicity, we will also adopt his notation here.

We proceed by induction: if $n = 1$, then the characteristic polynomial is $-\lambda$, so the claim holds. For $n = 2$, i.e. for the tree on 2 vertices, the characteristic polynomial is $\lambda^2 - 1$ (as we can check by direct computation), so the claim again holds, and we have our base case.

For the induction step, suppose that the above formula is true for all trees on up to $n - 1$ vertices. Let T be a tree on n vertices, let $p(\lambda)$ be its characteristic polynomial, and delete one of its leafs. If we now consider the original matchings in T, then there are two types of matchings that we can distinguish between: those that include the edge connecting the leaf to the rest of T and those that don't.

The matchings that include this edge cannot include any other edges incident to the leaf's neighbor, so these matchings correspond to the matchings in the tree with both the leaf and its neighbor deleted. Denote this graph by T'' and let its characteristic polynomial be $p_2(\lambda)$. Note that T'' need not be a tree: the second vertex that we delete might disconnect the tree. In this case, we use the fact that the characteristic polynomial of (however many) disconnected components is the product of the components' characteristic polynomials. In this case, the result follows from the exact same argument below (applied to the components), so in the following, we will assume that T'' is a tree. See Proposition 5.1 in [16] for details.

By induction hypothesis, the coefficient of the term with degree $(n-2)-2i$, call it c_i, is exactly the number of matchings of size i in T''. Once we count the deleted edge, we see that these matchings correspond to the matchings of size $i+1$ in T. By induction hypothesis, the term with coefficient c_i in $p_2(\lambda)$ has degree $(n-2)-2i$. But $(n-2)-2i = n-2(i+1)$, so the degree is the same as that of the term with coefficient a_{i+1} in $p(\lambda)$. Again by induction hypothesis, c_i has sign $(-1)^{n-2-i}$ in $p_2(\lambda)$, but a_{i+1} has sign $(-1)^{n-2(i+1)}$ in $p(\lambda)$, so $-p_2(\lambda)$ counts the number of matchings in T that include the edge incident to our leaf.

Now consider the matchings that do not contain the edge that connects our leaf to the rest of the tree. These can contain any of the other edges, hence correspond to matchings of size i in T'. Denote the characteristic polynomial of T' by $p_1(\lambda)$.

As before, it follows from our induction hypothesis that the coefficient of the term with degree $(n-1)-2i$ in $p_1(\lambda)$, call it b_i, is exactly the number of matchings of size i in T'. The corresponding degree of a_i in $p(\lambda)$ is $n-2i$. Considering the sign of a_i as before, we see that in $p(\lambda)$, a_i has sign $(-1)^{n-i}$, while the sign of b_i is $(-1)^{n-1-i}$. Thus, $-\lambda p_1(\lambda)$ counts the number of matchings in T that do not include the edge incident to our leaf.

In conclusion, we get that $p(\lambda) = -\lambda p_1(\lambda) - p_2(\lambda)$ counts the number of matchings in T.

$\square$

Before we return to Godsil, we require the following definition:

Definition 4.1.2. Let G be a graph with a unique perfect matching M and define the **quotient** or **contraction graph** G/M to be the graph obtained from G by contracting each edge of M onto a single vertex.

Then we have the following lemma due to Godsil:

Theorem 4.1.6. Let G be a bipartite graph with a unique perfect matching M, and let B be its Godsil matrix. If G/M is bipartite, then B^{-1} is diagonally similar to a non-negative integer matrix B^+, which dominates B, in the sense that $B^+ - B$ is a non-negative matrix. If G is a forest, then B^+ is a $(0,1)$-matrix.

We omit the proof of this result and instead focus on its immediate consequences: note that we may view the matrix B^+ as the incidence matrix of a (bipartite) multigraph, which we denote by G^+ and call the **inverse of** G. Also note that since B^+ dominates B, we can consider G as a spanning subgraph of G^+. Even more surprising, we can also show

Theorem 4.1.7. Let G be a forest with a unique perfect matching on $2k$ vertices, and let P_{2k} denote the path on $2k$ vertices. Then the graph inverse of G, G^+, is a spanning subgraph of P_{2k}^+.

Proof: Note that if $B = B(G)$, then B^+ is a $(0,1)$-matrix by the previous theorem. If $F_{2k} = B(P_{2k})$, then F_{2k}^+ is lower-triangular (assuming that the vertices of P_{2k} are labelled $1, k+1, 2, k+2, ...$), and each entry on the diagonal or below it is one. The result now follows by induction.

$\square$

We conclude this section with another useful result on the path on $2k$ vertices, which we will use in the next section to establish a lower bound on the LPE.

Theorem 4.1.8. Let $E = E_{2k}$ be the bipartite graph with $B = B(E)$ given by $B_{ij} = 0$ if $i < j$ or $i - j$ is even, and $B_{ij} = 1$ otherwise. Let G be a connected bipartite graph on $2k$ vertices, and assume that G has a unique perfect matching M and that its quotient graph G/M is bipartite. Let $B = B(G)$. Then $B(E)^+$ dominates B^+.

For a proof of this result, see [9].

4.1.2 Applications to the LPE

In this section, we apply our previous results on tree inverses to obtain bounds on the least positive eigenvalue of a tree on $2k$ vertices. Let G be a graph. Then we denote the i-th largest eigenvalue of G by $\lambda_i(G)$. As we observed in our numerical results in section 3.2, if G is a tree on $2k$ vertices, then the eigenvalues of $A(G)$ are symmetrically placed about the origin. Thus, $B = B(G)$ is invertible if and only if $\lambda_k(G) > 0$.

We now state Godsil's main result and show how it follows from the results in the previous section.

Theorem 4.1.9. Let G be a connected bipartite graph with a unique perfect matching M, such that the contraction graph G/M is bipartite, and suppose that $|G| = 2k$. Then

1. $\lambda_1(G)\lambda_k(G) \leq 1$, with equality if and only if $G = G^+$.
2. $\lambda_k(G) \geq \lambda_k(E_{2k})$, with equality if and only if $G \approx E_{2k}$.
3. If G is a forest $\lambda_m(G) \geq \lambda(P_{2k})$, with equality if and only if $G \approx P_{2k}$.

Proof: By Theorem 4.1.6, B^+ is similar to B^{-1}, so $\lambda_1(G^+) = 1/\lambda_1(G)$. B^+ dominates B, so $\lambda_1(G) \leq \lambda_1(G^+)$, which proves the first claim.

From 4.1.8, we see that $B(E_{2k}^+)$ dominates B^+, so $1/\lambda_m(G) \leq 1/\lambda_m(E_{2m})$, from which the second claim follows.

Finally, from 4.1.7 we know that if G is a forest, then $B(P_{2m})^+$ dominates B^+, so the last claim follows.

□

It follows that the LPE over all trees of size $2k$ occurs on the $2k$-path. From this, we can explicitly compute the LPE (see section 4.2.2).

4.1.3 Generalizing Godsil

Given the success of Godsil's method involving tree inverses, it seems only natural to ask what results might carry over to the odd case. In this section, we will try to generalize several of Godsil's results and show why it seems difficult to apply them to the odd case. This will motivate our investigation of another approach - characteristic polynomials of trees - in the next section.

Theorem 4.1.9 relies on Theorems 4.1.6, 4.1.7, and 4.1.8 being true. Let us begin by generalizing 4.1.6 to the odd case. Let G be a bipartite graph on $2k+1$ vertices. It is easy to see that a graph with a unique perfect matching (UPM) must have an even number of vertices, so G has no UPM M, and hence there can be no contraction graph G/M.

The question then becomes whether we might be able to work without these assumptions, perhaps prove a slightly weaker result than that B^{-1} (where B is the Godsil matrix) is diagonally similar to a non-negative integer matrix B^+. The answer, however, is no, since B^{-1} is not even well-defined. Consider the following example.

Counterexample 4.1.1. Let G be the star on 5 vertices, let v_1 be the center of the star, and denote the other vertices by $v_2, ..., v_5$. Then $V_1 = \{v_2, ..., v_5\}$, $V_2 = \{v_1\}$ is a bipartition of G and the Godsil matrix is given by

$$B(G) = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

which is obviously not invertible, so we cannot speak of B^{-1}, let alone B^+. 4.1.7 and 4.1.8 rely on the existence of B^+, so if we cannot guarantee that B^+ exists, then it is unclear how we should attempt to generalize these results.

4.2 Characteristic Polynomials for Trees

In the previous section, we saw that while Godsil's method can be used to find the LPE of a tree on an even number of vertices, it is difficult to generalize it to the odd case. In this section, we present a different approach first investigated by Spiridonov in [16].

After briefly elaborating on Spiridonov's results, we will show how one of our own results (previously presented in section 4.1.1, where we used it to prove one of Godsil's claims) can be used to prove several of Spiridonov's conjectures. We will then assume that the LPE of a $2k+1$-vertex tree occurs on the $2k$ forked path and explicitly compute the eigenvalue. We will then conclude this section - and thereby the chapter - with a summary of our ideas on how to use our results to prove that the LPE indeed occurs on the $2k$ forked path.

4.2.1 Characteristic Polynomials of Adjacency Matrices

In the following, when we refer to the characteristic polynomial of a graph G, we mean the characteristic polynomial of the adjacency matrix $A(G)$ introduced earlier. We denote the coefficient of the x^i term of the characteristic polynomial by a_i.

Spiridonov, focusing on the even case, is able to prove that

Theorem 4.2.1. If a tree has size $2k$ and $a_0 \neq 0$, then $|a_0| = 1$.

This, however, cannot be generalized to the odd case, i.e. it is not true that

"If a tree has odd size and $a_1 \neq 0$, then $|a_1| = 1$."

as the following example shows.

Counterexample 4.2.1. Let G be the walk on 5 vertices. Then

$$|A(G) - xI| = \begin{vmatrix} -x & 1 & 0 & 0 & 0 \\ 1 & -x & 1 & 0 & 0 \\ 0 & 1 & -x & 1 & 0 \\ 0 & 0 & 1 & -x & 1 \\ 0 & 0 & 0 & 1 & -x \end{vmatrix} = -x^5 + 4x^3 - 3x$$

Spiridonov further conjectures that

Conjecture 4.2.1. The minimum possible magnitude of any $A_i \neq 0$ for the characteristic polynomial of a tree is exactly $i + 1$.

While we cannot prove this, we can see that it at least holds numerically (see the appendix for our numerical results). Based on this, Spiridonov deduces that trees of size $2k + 1$ need not necessarily have a lower LPE than trees of size $2k$. We can improve upon this result and show the following:

Theorem 4.2.2. Let T be a tree of size n with LPE λ_T and at least one zero eigenvalue. Then there exists a tree T' of size $n - 1$ with LPE $\lambda_{T'} \leq \lambda_T$.

Note that the above implies Spiridonov's conjecture, since the symmetry of the tree spectrum implies the existence of a zero-eigenvalue for odd trees. We require the following lemma due to Cauchy:

Lemma 4.2.3. Let M be a Hermitian $n \times n$ matrix with eigenvalues $\lambda_1 \leq ... \leq \lambda_n$. Let M' be any $(n-1) \times (n-1)$ minor of M with eigenvalues $\sigma_1 \leq ... \leq \sigma_{n-1}$. Then $\lambda_1 \leq \sigma_1 \leq \lambda_2 \leq \sigma_2 \leq ... \leq \sigma_{n-1} \leq \lambda_n$.

Proof of the Claim: Let T be a tree on m vertices and suppose that T has j zero eigenvalues. Then T has a matching of size $\frac{m-j}{2}$. We know that at least one vertex is not included in the matching. Suppose that this vertex is a leaf.

Deleting this vertex, we get the graph T', which still has a matching of size $\frac{m-j}{2}$. Note that $A(T')$ is a principal minor of $A(T)$, so that by Cauchy,

$$0 \leq \lambda_{T'} \leq \lambda_T \leq ...$$

Suffice it to show that our leaf assumption is justified, i.e. that there exists a matching with an excluded leaf.

Suppose only non-leaf vertices are excluded from the matching. Choose an unmatched vertex and consider a path from this vertex to a matched leaf. If there is another unmatched (non-leaf) vertex along this path, consider this vertex instead. Invert the matching along this path and note that this is still a matching, since the initial vertex was not in the matching. Hence we can always find a matching with an excluded leaf.

□

We can further use Theorem 4.1.5, which we established in section 4.1.1, to prove another one of Spiridonov's conjectures.

Theorem 4.2.4. For a characteristic polynomial of a tree of size k, $|a_i| \leq \binom{k-i}{i}$. The maximum is achieved for every i by the k-walk.

Proof: We can in fact prove this for any forest on k vertices. First note that the number of matchings of size i in the k-path is $\binom{k-i}{i}$. Suffice it to show that this is the maximum:

We proceed by induction on k: if $k = 1$, then this is trivial, so the base case holds. Suppose that the claim holds for trees of size 1 up to $k-1$, i.e. the number of matchings of size i is less than or equal to $\binom{k-i-1}{i}$. Let P_k be the k path and let T be any other tree. Choose a leaf in each and count the matchings of size i in each graph that include this leaf and those that don't.

For the first category, delete the edge that connects this leaf to the rest of the graph and its two vertices and count the matchings of size $i-1$ in the remaining graph. Note that P_k becomes P_{k-2}, while T becomes a forest T' on $k-2$ vertices. By induction hypothesis, the number of matchings of size $(i-1)$ in P_{k-2} is larger than or equal to the number of matchings in T', so the claim holds.

For the second category, again delete the leaf and the edge that connects it to the rest of the tree. This time, we count the number of matchings of size i in the remaining graphs: P_k becomes P_{k-1} and T becomes a forest of size $k-1$. The claim again follows from the induction hypothesis.

□

Spiridonov further suggests that in order to prove that the (forked) path produces the LPE, we need to have control over the ratios $\frac{a_{i+2}}{a_i}$. The control over the ratios that Theorem 4.2.1 and Theorem 4.2.4 give us seems insufficient [16].

Based on our numerical results in section 3.2, we make the following conjectures on non-zero coefficients.

Conjecture 4.2.2. Let r_i denote the maximum ratio between the coefficients a_{i+2} and a_i, where a_j are the coefficients of the characteristic polynomial of a tree of size $\geq j$. Then

$$|r_{2k}| \geq |r_{2k+1}|$$

i.e. the maximum ratio on all trees on $2k$ vertices dominates the maximum ratio on all trees on $2k+1$ vertices.

Conjecture 4.2.3. For each number of vertices k, the maximum ratio occurs on the k-path, while the minimum occurs on the k-star.

Conjecture 4.2.4. For each number of vertices k, the maximum (resp. minimum) is unique.

Since we are assuming the coefficients to be non-zero, we can use our result on the maximum coefficients in Theorem 4.2.4 to conjecture the following upper bound on the ratios:

Conjecture 4.2.5. Using the same notation as in Conjecture 4.2.2,

$$\max_{0\leq i\leq k-2}\left|\frac{\binom{k-i-2}{i-2}}{\binom{k-i}{i}}\right| \geq |r_{2k}|$$

4.2.2 Computing the LPE

In this section, we assume that the LPE over all trees of size $2k$ occurs on the $2k$ path and explicitly compute the LPE of a tree on $2k$ vertices. Similarly for the LPE over all trees of size $2k+1$ occurring on the $2k$ forked path, where we provide a partial proof.

Theorem 4.2.5. The least positive eigenvalue of a $2k$-path is $2\cos\left(\frac{\pi n}{2n+1}\right)$

Proof: We will argue by analogy with section 5.2.3 in [16] and show that all eigenvalues of the n-path are of the form

$$2\cos\left(\frac{k\pi}{n+1}\right)$$

for $k = 1, ...n$, from which the result follows.

Denote the characteristic polynomial of the n-path by p_n. Then we know from Spiridonov that for $n \geq 1$,

$$p_n(\lambda) = \lambda p_{n-1}(\lambda) - p_{n-2}(\lambda)$$

where we let $p_1(\lambda) = 0$ and $p_{-1}(\lambda) = 0$. Solving the recurrence relation and finding the roots of the corresponding polynomial $x^2 - \lambda x + 1 = 0$, we get that

$$x_1 = \frac{\lambda + \sqrt{\lambda^2 - 4}}{2}, x_2 = \frac{\lambda - \sqrt{\lambda^2 - 4}}{2}$$

which implies

$$p_n(\lambda) = c_1 x_1^{n+1} + c_2 x_2^{n+1}$$

Let $n = 0$ and -1 to get that

$$c_1 + c_2 = 0 \text{ and } c_1 x_1 + c_2 x_2 = 1$$

from which it follows that

$$p_n(\lambda) = \frac{1}{\sqrt{\lambda^2 - 4}}(x_1^{n+1} - x_2^{n+1})$$

Now if $p_n(\lambda) = 0$, then $x_1^{n+1} = x_2^{n+1}$, or equivalently,

$$x_1 = e^{\frac{2k\pi i}{n+1}} x_2$$

for $0 \leq k \leq n$. Solving for λ, we get that

$$\lambda = \pm \left(e^{\frac{k\pi i}{n+1}} + \frac{1}{e^{\frac{k\pi i}{n+1}}} \right) = \pm 2 \cos \frac{k\pi}{n+1}$$

Note that we may simply write

$$2\cos\frac{k\pi}{n+1}$$

since $-\cos\frac{k}{n+1} = \cos\frac{n+1-k}{n+1}$, so the result follows.

□

We proceed by analogy with the above to prove the odd case:

Theorem 4.2.6. The least positive eigenvalue of a tree on $2n+1$ vertices is $2\cos\left(\frac{\pi(2n-1)}{4n}\right)$.

Proof: Let $b_1, ..., b_{2n+1}$ be eigenfunctions of the eigenvalue λ for the forked $2n$ path. Then we have the following constraints:

1. For $k = 3, ..., 2n-1$, $\lambda b_{k+1} = b_k + b_{k+2}$,
2. $b_3 = \lambda b_1$,
3. $b_3 = \lambda b_2$,
4. $b_{2n} = \lambda b_{2n+1}$,
5. $b_1 + b_2 + b_4 = \lambda b_3$

From (2) and (3), we get that $b_1 = b_2$. Suppose $b_1 = b_2 = 0$. Then $b_3 = 0$ from (2) and (3). $b_4 = 0$ from (5), and $b_5 = b_6 = ... = 0$ from (1), so $b_2, b_1 \neq 0$. Thus we may normalize and set $b_1 = b_2 = 1$, $b_3 = \lambda$, and $b_4 = \lambda^2 - 2$. Solving the recurrence in (1), we get

$$b_k = c_1 x_1^k + c_2 x_2^k$$

where

$$x_1 = \frac{\lambda + \sqrt{\lambda^2 - 4}}{2}, x_2 = \frac{\lambda - \sqrt{\lambda^2 - 4}}{2}$$

From this, we get the following two restrictions:

1. $c_1 x_1 + c_2 x_2 = 1$,
2. $c_1 x_1^2 + c_2 x_2^2 = 1$

From (1), we get

$$(c_1 + c_2)\lambda + (c_1 - c_2)\sqrt{\lambda^2 - 4} = 2$$

and from (2), we have

$$c_1(\lambda^2 + 2\lambda\sqrt{\lambda^2 - 4} + \lambda^2 - 4) + c_2(\lambda^2 - 2\lambda\sqrt{\lambda^2 - 4} + \lambda^2 - 4) = 4$$

which then implies

$$2\lambda((c_1 + c_2)\lambda + (c_1 - c_2)\sqrt{\lambda^2 - 4}) - 4(c_1 + c_2) = 4$$

Simplifying, we get that

$$c_1 = \frac{2 - (\lambda - 4)\lambda}{2\sqrt{\lambda^2 - 4}} + \frac{\lambda}{2} - 2$$

$$c_2 = -\frac{2 - (\lambda - 4)\lambda}{2\sqrt{\lambda^2 - 4}} + \frac{\lambda}{2} - 2$$

Condition (1) then implies that

$$p_n(\lambda) = \left(\frac{2 - (\lambda - 4)\lambda}{2\sqrt{\lambda^2 - 4}} + \frac{\lambda}{2} - 2 \right) x_1 - \left(\frac{2 - (\lambda - 4)\lambda}{2\sqrt{\lambda^2 - 4}} - \frac{\lambda}{2} + 2 \right) x_2$$

From this, it should be possible to show that

$$x_1 = e^{\frac{(2k-1)\pi i}{n}} x_2 \, , 1 \leq n$$

from which the result then follows by the exact same argument as in the even case.

□

4.2.3 Directions for Future Research

In this section, we conclude our discussion of the LPE and of the papers of Godsil and Spiridonov, by presenting possible directions for future research.

The most natural next step would be to prove our conjectures on the ratios of the coefficients of the characteristic polynomial of the adjacency matrix of a tree in section 4.2.1. For this, Theorem 4.2.4 should be useful, and the proof(s) should most likely proceed along lines similar to those in the proof of 4.2.4. The major obstacle in this direction will be how to use the coefficient ratios to prove that the LPE indeed occurs on the $2k$ path, resp. on the $2k$ forked path. Once we know how to do this, the proof of the odd case then follows readily from Theorem 4.2.6.

Another possible, although somewhat less promising, avenue of investigation might be found in section 4.1.3. While we are currently unable to generalize Godsil's results in a direct way, there are several questions here that might be worth considering: is it necessary to consider the inverse of the incidence matrix due to Godsil (B^{-1}), or would a pseudo-inverse be enough? Could this lead to a more general notion of a tree inverse, and could this lead to results similar to those in Godsil, but general enough to include trees on an odd number of vertices? Is it necessary to restrict ourselves to graphs with a unique perfect matching, or is an almost perfect matching (i.e. a perfect matching that excludes exactly one vertex) good enough?

4.3 Conclusion

The work of Godsil on tree inverses has provided us with a combinatorial proof for the occurrence of the least positive eigenvalue of a tree on $2k$ vertices on the $2k$ path. In this project, we saw why it seems challenging to generalize these results to trees on $2k + 1$ vertices.

Following an idea first proposed by Spiridonov, we used the characteristic polynomials of tree adjacency matrices to approach this case. We improved upon Spiridonov's results by showing that the LPE on $2k$ vertices lower bounds the LPE on $2k + 1$ vertices, and used a new theorem on the form of the characteristic polynomial to prove several of Spiridonov's conjectures.

Based on our numerical results, we made several conjectures of our own on the coefficient ratios of the characteristic polynomial. If we can prove these conjectures and use them to show that the LPE occurs on the forked $2k$ path, the result follows. We presented several strategies on how to bridge this gap in our discussion of possible directions for future research, which makes us hopeful that we are now closer to a proof of the odd case.

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Appendix A

Access to Numerical Results

All the numerical results mentioned in this capstone and the MATLAB code that generated them are available at

https://github.com/LFesser97/Spectral-Distributions-of-Sparse-Random-Graphs-and-Matrices

In order to navigate the repository, we ask the reader to consult the file README.md available under the above link.