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Author
Tobin, Robin Joshua

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Extremal Spectral Invariants of Graphs

A dissertation submitted in partial satisfaction of the
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in

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by

Robin Joshua Tobin

Committee in charge:

Professor Fan Chung Graham, Chair
Professor Jacques Verstraëte, Co-Chair
Professor Ronald Graham
Professor Ramamohan Paturi
Professor Jeffrey Remmel

2017

The dissertation of Robin Joshua Tobin is approved, and it is acceptable in quality and form for publication on microfilm and electronically:

Co-Chair

Chair

University of California, San Diego

2017

DEDICATION

To my family (be they Tobins, Dohertys or Ryans).

EPIGRAPH

Shut up!

I am working Cape Race.

—Jack Phillips

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VITA

2011	B. A. in Mathematics, The University of Dublin, Trinity College.
2013	M. A. in Mathematics, University of California, San Diego.
2017	Ph. D. in Mathematics, University of California, San Diego.

ABSTRACT OF THE DISSERTATION

Extremal Spectral Invariants of Graphs

by

Robin Joshua Tobin

Doctor of Philosophy in Mathematics

University of California, San Diego, 2017

Professor Fan Chung Graham, Chair
Professor Jacques Verstraëte, Co-Chair

We address several problems in spectral graph theory, with a common theme of optimizing or computing a spectral graph invariant, such as the spectral radius or spectral gap, over some family of graphs. In particular, we study measures of graph irregularity, we bound the adjacency spectral radius over all outerplanar and planar graphs, and finally we determine the spectral gap of reversal graphs and a family of graphs that generalize the prefix reversal graph.

Firstly we study two measures of graph irregularity, the principal ratio and the difference between the spectral radius of the adjacency matrix and the average degree.

For the principal ratio, we show that the graphs which maximize this statistic are the *kite graphs*, which are a clique with a pendant path, when the number of vertices is sufficiently large. This answers a conjecture of Cioabă and Gregory. For the second graph irregularity measure, we show that the connected graphs which maximize it are *pineapple graphs*, answering a conjecture of Aouchiche et al.

Secondly we investigate the maximum spectral radius of the adjacency matrix over all graphs on n vertices within certain well-known graph families. Our main result is showing that the planar graph on n vertices with maximal adjacency spectral radius is the join $P_2 + P_{n-2}$, when n is sufficiently large. This was conjectured by Boots and Royle. Additionally, we identify the outerplanar graph with maximal spectral radius, answering a conjecture of Cvetkoviȁ and Rowlinson.

Finally, we determine the spectral gap of various Cayley graphs of the symmetric group S_n, which arise in the context of substring reversals. This includes an elementary proof that the prefix reversal (or *pancake flipping* graph) has spectral gap one, originally proved via representation theory by Cesi. We generalize this by showing that a large family of related graphs all have unit spectral gap.

Chapter 1

Introduction

1.1 Preliminaries

The subject of this dissertation is *spectral graph theory*, which studies graphs through various associated matrices, such as the adjacency matrix or normalized Laplacian. We will address several problems in this area, with a common theme of computing or maximizing a spectral parameter, such as the spectral radius, over some families of graphs. In this section, we provide an overview of the background terminology and results that will be used throughout the dissertation, and establish notation. The section concludes with a summary of the main results.

A graph G is a pair (V,E), where V is a set of *vertices* and E is a set of unordered pairs of vertices, which are called the *edges* of G. When the underlying graph is not clear from context, we will use the notation $V = V(G)$ and $E = E(G)$. A subgraph of G is a graph whose vertex set and edge set are subsets of $V(G)$ and $E(G)$ respectively.

Two vertices x, y are said to be *adjacent* if the pair (x, y) belongs to the edge set. The *neighbors* of a vertex x, denoted $N(x)$, is the set of all vertices that are adjacent to x. The *degree* of a vertex x, denoted d_x, is defined by $d_x = |N(x)|$. The *average degree* d of a graph is then given by

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

A graph is *d-regular* if every vertex has degree d.

1.2 Spectral graph theory

1.2.1 Matrices associated to graphs

Given a graph G on n vertices, many $n \times n$ matrices which encode the structure of the graph have been studied, including the adjacency matrix A, the combinatorial Laplacian L, the normalized Laplacian $\mathcal{L}$, the distance matrix D [29] and the signless Laplacian Q [18]. We will be concerned with three of these, the adjacency matrix, and the combinatorial and normalized Laplacians. In this subsection we define these matrices, and discuss some of their properties. Throughout this subsection we will be considering a graph G with vertex set $V(G) = \{1, 2, \cdots, n\}$.

The adjacency matrix is the $n \times n$ matrix defined by

$$A(i,j) = \begin{cases} 1 & \text{if } (i,j) \text{ is an edge of } G \\ 0 & \text{if } (i,j) \text{ is not an edge of } G. \end{cases}$$

This is a symmetric matrix, and so will have n real eigenvalues and a basis of n orthogonal eigenvectors. We will denote the eigenvalues of the adjacency matrix by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. By the Perron–Frobenius theorem, if the graph G is connected then $\lambda_1 > \lambda_2$, and we can choose eigenvector corresponding to λ_1 whose entries are all strictly positive.

The combinatorial Laplacian is defined by $L = D - A$, where D is the diagonal matrix with $D(i,i) = d_i$. The eigenvalues of this matrix are non-negative, which follows easily from considering the the eigenvector entry of largest absolute value (or alternatively, it is an immediate consequence of the Gershgorin circle theorem [36]). The smallest eigenvalue of this matrix is 0, and the corresponding eigenvector is the constant vector. The normalized Laplacian $\mathcal{L}$ is defined by $\mathcal{L} = D^{-1/2}LD^{-1/2}$. The eigenvalues of the normalized Laplacian lie between 0 and 2.

For real symmetric matrices, we have the following characterization for all of its eigenvalues.

Theorem 1.2.1 (Courant–Fischer for real matrices)**.** *Let A be a real symmetric matrix, with eigenvalues* $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$*. For any* $1 \leq k \leq n$*, we have*

$$\min_{w_1,w_2,\cdots,w_{n-k}\in\mathbb{R}^n} \max_{\substack{x\neq 0, x\in\mathbb{R}^n \\ x\perp w_1,w_2,\cdots,w_{n-k}}} \frac{x^TAx}{x^Tx} = \lambda_k,$$

and

$$\max_{w_1,w_2,\cdots,w_{k-1}\in\mathbb{R}^n} \min_{\substack{x\neq 0, x\in\mathbb{R}^n \\ x\perp w_1,w_2,\cdots,w_{k-1}}} \frac{x^TAx}{x^Tx} = \lambda_k.$$

As a special case, we recover the Rayleigh–Ritz characterization of the extremal eigenvalues λ_1 and λ_n,

Theorem 1.2.2 (Rayleigh–Ritz for real matrices)**.** *Let A be a real symmetric matrix, with eigenvalues* $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$*.*

$$\lambda_1 = \max_{x\neq 0} \frac{x^TAx}{x^Tx},$$

and

$$\lambda_n = \min_{x\neq 0} \frac{x^TAx}{x^Tx}.$$

For the adjacency matrix, that yields the following characterization of the largest eigenvalue,

$$\lambda_1 = \max_{x\neq 0} \frac{x^TAx}{x^Tx} = \max_{x\neq 0} \frac{2\sum_{(i,j)\in E(G)} x_i x_j}{x^Tx}.$$

1.2.2 Fundamental inequalities

We will frequently manipulate inequalities involving properties of the graph, such as the number of edges, and spectral parameters, such as the eigenvalues and eigenvector entries. We introduce such manipulations by giving the proofs of some classic inequalities in spectral graph theory which we will use.

Throughout this section we will assume that $\mathbf{v}$ is the eigenvector corresponding to the eigenvalue λ_1 of the adjacency matrix. Additionally we assume that it is normalized so that it has maximum entry equal to 1, and that vertex x is a vertex attaining this. From the definition of the adjacency matrix, we have

$$\lambda_1 \mathbf{v}_y = \sum_{z \sim y} \mathbf{v}_z. \tag{1.1}$$

Our choice of normalization yields

$$\lambda_1 \mathbf{v}_y = \sum_{y \sim x} \mathbf{v}_y \leq d_y. \tag{1.2}$$

Theorem 1.2.3 (Stanley [49]). *Given a graph G with m edges and largest adjacency eigenvalue λ_1, we have*

$$\lambda_1 \leq \frac{-1+\sqrt{8m+1}}{2},$$

with equality only when G is the union of a complete graph and a (possibly empty) independent set of vertices.

Proof. We have

$$\lambda_1^2 = \lambda_1^2 \mathbf{v}_x \quad = \quad \sum_{y \sim x} \lambda_1 \mathbf{v}_y \leq \sum_{y \sim x} d_y \leq 2m - d_x \leq 2m - \lambda_1,$$

where the last inequality follows from $\lambda_1 \leq d_x$. This implies the desired inequality. For the equality case, we must have $\lambda_1 = d_x$ and $\sum_{y\sim x} d_y = 2m - d_x$. This happens only if every edge in G is incident to a vertex in $N(x)$, and if there is a d_x-regular connected component. This is exactly the union of a complete graph and an independent set of vertices.

□

There have been many generalizations of this result [25, 53, 35, 44, 19], as well as several similar inequalities, which incorporate additional information about the graph structure such as the minimum or maximum degree [23, 7, 46]. We highlight one of these generalizations here, which we will have occasion to use later.

Theorem 1.2.4 (Hong [53]). *Given a connected graph G with m edges and largest adjacency eigenvalue λ_1, we have*

$$\lambda_1 \leq \sqrt{2m - n + 1},$$

with equality only when G is either K_n or $K_{1,n}$.

This can be proved with a small modification to the proof above.

1.3 Overview of results

The remainder of this thesis is broken into three chapters. In Chapter 2 we consider measures of graph irregularity, which are statistics that quantify how much a graph deviates from being regular. In particular, we consider two such statistics. The first is the principal ratio, which, for a connected graph, is the ratio of the largest and smallest entries of the leading eigenvector of the adjacency matrix. For this statistic, we characterize the extremal graphs for large enough n. This was conjectured by Cioabă and Gregory [16].

Theorem 1.3.1. *For sufficiently large n, the connected graph G on n vertices with largest principal ratio is a kite graph.*

The second graph irregularity measure we consider is $\lambda_1 - d$, the difference between the largest adjacency eigenvalue and the average degree. In this case we show that the extremal connected graphs are *pineapple graphs*, which are a clique with a set of pendant edges added to a single vertex on the clique. This was conjectured by Aouchiche et al [4].

Theorem 1.3.2. *For sufficiently large n, the connected graph that maximizes $\lambda_1 - d$ is a pineapple graph.*

In Chapter 3, we consider planar and outerplanar graphs, and maximize the adjacency spectral radius over each of these families for a fixed number of vertices. The problem of determining the maximum spectral radius over some family of geometric graphs has been studied by many authors, with the case of planar graphs receiving particular attention. We show that for sufficiently large n the extremal graphs are the graphs $P_2 + P_{n-2}$. This was conjectured independently by Boots and Royle in 1991 [8] and by Cao and Vince in 1993 [11].

Theorem 1.3.3. *For sufficiently large n, the planar graph on n vertices that maximizes λ_1 is $P_2 + P_{n-2}$.*

We also answer the analogous problem for outerplanar graphs, showing that the extremal graph in that case is given by $P_1 + P_{n-1}$, as conjectured by Cvetković and Rowlinson [17].

Theorem 1.3.4. *For sufficiently large n, the outerplanar graph on n vertices that maximizes λ_1 is $P_1 + P_{n-1}$.*

Finally, in Chapter 4 we study several families of graphs that arise in the context of *substring reversals*. Given a permutation σ written in list notation $(\sigma_1, \sigma_2, \cdots, \sigma_n)$, a substring reversal is any permutation of the form

$$(\sigma_1, \sigma_2, \cdots, \sigma_{i-1}, \sigma_j, \sigma_{j-1}, \cdots, \sigma_i, \sigma_{j+1}, \cdots, \sigma_n).$$

When $i = 1$, this is a *prefix reversal*. The *reversal graph* has vertex set S_n and where two vertices are adjacent if they can be obtained from one another by a substring reversal. The study of this graph is motivated by applications in mathematical biology [5]. Our main result is determining the spectral gap of this graph.

Theorem 1.3.5. *Let λ_1, λ_2 be the largest and second largest eigenvalues of the adjacency matrix of the reversal graph. Then $\lambda_1 - \lambda_2 = n$.*

Additionally, we construct a family of graphs which generalize the prefix reversal graph, for which every graph has spectral gap equal to one. This provides a combinatorial proof that the spectral gap of the prefix reversal gap is one, which was proved via representation theory by Cesi [12], who in turn was answering a question posed by Gunnells, Scott and Walden [31].

Chapter 2

Measures of graph irregularity

2.1 Introduction

A *measure of graph irregularity* is a statistics that quantifies how far a graph is from being regular. The choice of the word "measure" is slightly unfortunate due to its more common alternative meaning, but this is the phrase that has been used repeatedly in the literature, and so we adopt it here. Many different such statistics have been proposed. There is the *irregularity of a graph* as defined by Albertson [3],

$$\mathrm{irr}(G) = \sum_{(u,v)\in E(G)} |d_u - d_v| \,.$$

A variant of this that depends only on the degree sequence of a graph, the *total irregularity*, was introduced by Abdo et. al. [1],

$$\mathrm{irr}_{\mathrm{it}}(G) = \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} |d_u - d_v|$$

Another irregularity measure that does depends only on the degree sequence is given by the variance of the degree sequence, studied by Bell [6],

$$var(G) = \frac{1}{n} \sum_{v \in V(G)} |d_v - d|^2 .$$

Collatz and Sinogowitz, in perhaps the first spectral graph theory paper, noted that the difference between the largest adjacency eigenvalue and the average degree can be seen as a measure of the irregularity of a connected graph [52]. Finally, the *principal ratio* of a connected graph was studied as a measure of graph irregularity by Cioabă and Gregory [16],

$$\gamma(G) = \frac{\mathbf{x}_{\max}}{\mathbf{x}_{\min}},$$

where $\mathbf{x}$ is a positive eigenvector corresponding to the largest eigenvalue of the adjacency matrix, and $x_{\min}$ and $x_{\max}$ are the smallest and largest eigenvector entries respectively.

In this section we determine the extremal graphs with respect to the last two irregularity measures, answering conjectures of Cioabă and Gregory [16] and Aouchiche et. al. [4].

Let $P_r \cdot K_s$ be the graph attained by identifying an end vertex of a path on r vertices to any vertex of a complete graph on s vertices. This has been called a *kite graph* or a *lollipop graph*. Cioabă and Gregory [16] conjectured that the connected graph on n vertices maximizing γ is a kite graph. Our first result proves this conjecture for n large enough.

Theorem 2.1.1. *For sufficiently large n, the connected graph G on n vertices with largest principal ratio is a kite graph.*

A *pineapple graph* is a clique with pendant edges added to a single vertex. Aouchiche et al [4] conjectured that the extremal connected graph with respect to the invariant $\lambda_1 - d$ is a pineapple graph. We show this for sufficiently large n.

Theorem 2.1.2. *For sufficiently large n, the connected graph G on n that maximizes $\lambda_1 - d$ is a pineapple graph.*

An analogous problem for directed graphs, finding graphs which maximize the principal ratio for directed graphs, was answered by Aksoy et al [2]. We note that Brightwell and Winkler [9] showed that a kite graph maximizes the expected hitting time of a random walk. The extremal graphs for various of these irregularity measures have been studied. The extremal graphs with respect to $\mathrm{irr}(G)$ were characterized by Hansen and Mélot [33], and the extremal graphs with respect to the total irregularity were studied by [1]. Nikiforov [45] proved several inequalities comparing $var(G)$, $\varepsilon(G)$ and $s(G) := \sum_v |d(u) - d|$. Bell showed that $\varepsilon(G)$ and $var(G)$ are incomparable in general [6]. Finally, additional bounds on $\gamma(G)$ have been given in [16, 47, 43, 40, 56].

2.2 Graphs of maximal principal ratio

2.2.1 Structural lemmas

Throughout this section G will be a connected simple graph on n vertices. The eigenvectors and eigenvalues of G are those of the adjacency matrix A of G. The vector $\mathbf{v}$ will be the eigenvector corresponding to the largest eigenvalue λ_1, and we take $\mathbf{v}$ to be scaled so that its largest entry is 1. Let x_1 and x_k be the vertices with smallest and largest eigenvector entries respectively, and if several such vertices exist then we pick any of them arbitrarily. Let $x_1, x_2, \cdots, x_k$ be a shortest path between x_1 and x_k. Let $\gamma(G)$ be the principal ratio of G.

Recall that the vertices $v_1, v_2, \cdots, v_m$ are a *pendant path* if the induced graph on these vertices is a path and furthermore if, in G, v_1 has degree 1 and the vertices

$v_2, \cdots, v_{m-1}$ have degree 2 (note there is no requirement on the degree of v_m).

Lemma 2.2.1. *If $\lambda_1 \geq 2$ and $\sigma = (\lambda_1 + \sqrt{\lambda_1^2 - 4})/2$, then for $1 \leq j \leq k$,*

$$\gamma(G) \leq \frac{\sigma^j - \sigma^{-j}}{\sigma - \sigma^{-1}} \mathbf{v}_{x_j}^{-1}.$$

Moreover we have equality if the vertices $x_1, x_2, \cdots, x_j$ are a pendant path.

Proof. We have the following system of inequalities

$$\begin{aligned}
\lambda_1 \mathbf{v}_{x_1} &\geq \mathbf{v}_{x_2} \\
\lambda_1 \mathbf{v}_{x_2} &\geq \mathbf{v}_{x_1} + \mathbf{v}_{x_3} \\
\lambda_1 \mathbf{v}_{x_3} &\geq \mathbf{v}_{x_2} + \mathbf{v}_{x_4} \\
\vdots \quad & \quad \vdots \\
\lambda_1 \mathbf{v}_{x_{j-1}} &\geq \mathbf{v}_{x_j} + \mathbf{v}_{x_{j-2}}.
\end{aligned}$$

The first inequality implies that

$$\mathbf{v}_{x_1} \geq \frac{1}{\lambda_1} \mathbf{v}_{x_2}.$$

Plugging this into the second equation and rearranging gives

$$\mathbf{v}_{x_2} \geq \frac{\lambda_1}{\lambda_1^2 - 1} \mathbf{v}_{x_3}.$$

Now assume that

$$\mathbf{v}_{x_i} \geq \frac{u_{i-1}}{u_i} \mathbf{v}_{x_{i+1}},$$

with some positive constants u_j for all $j < i$. Then

$$\lambda_1 \mathbf{v}_{x_{i+1}} \geq \mathbf{v}_{x_i} + \mathbf{v}_{x_{i+2}}$$

implies that

$$\mathbf{v}_{x_{i+1}} \geq \frac{u_i}{\lambda_1 u_i - u_{i-1}} \mathbf{v}_{x_{i+2}},$$

where $\lambda_1 u_i - u_{i-1}$ must be positive because $\mathbf{v}_{x_j}$ is positive for all j. Therefore the coefficients u_i satisfy the recurrence

$$u_{i+1} = \lambda_1 u_i - u_{i-1}$$

Solving this and using the initial conditions $u_0 = 1$, $u_1 = \lambda$ we get

$$u_i = \frac{\sigma^{i+1} - \sigma^{-i-1}}{\sigma - \sigma^{-1}}$$

In particular, u_i is always positive, a fact implicitly used above. Finally this gives,

$$\mathbf{v}_{x_1} \geq \frac{u_0}{u_1} \mathbf{v}_{x_2} \geq \frac{u_0}{u_1} \cdot \frac{u_1}{u_2} \mathbf{v}_{x_3} \geq \cdots \geq \frac{\mathbf{v}_{x_j}}{u_{j-1}}$$

Hence

$$\gamma(G) = \frac{\mathbf{v}_{x_k}}{\mathbf{v}_{x_1}} = \frac{1}{\mathbf{v}_{x_1}} \leq \frac{\sigma^j - \sigma^{-j}}{\sigma - \sigma^{-1}} \mathbf{v}_{x_j}^{-1}$$

If these vertices are a pendant path, then we have equality throughout. □

We will also use the following lemma which comes from the paper of Cioabă and Gregory [16].

Lemma 2.2.2. *For $r \geq 2$ and $s \geq 3$,*

$$s - 1 + \frac{1}{s(s-1)} < \lambda_1(P_r \cdot K_s) < s - 1 + \frac{1}{(s-1)^2}.$$

In the remainder of the section we prove Theorem 2.1.1. We now give a sketch of the proof that is contained in Section 2.2.2.

1. We show that the vertices $x_1, x_2, \cdots, x_{k-2}$ are a pendant path and that x_k is connected to all of the vertices in G that are not on this path (lemma 2.2.4).

2. Next we prove that the length of the path is approximately $n - n/\log(n)$ (lemma 2.2.5).

3. We show that x_{k-2} has degree exactly 2 (lemma 2.2.8), which extends our pendant path to $x_1, x_2, \cdots, x_{k-1}$. To do this, we find conditions under which adding or deleting edges increases the principal ratio (lemma 2.2.6).

4. Next we show that x_{k-1} also has degree exactly 2 (lemma 2.2.10). At this point we can deduce that our extremal graph is either a kite graph or a graph obtained from a kite graph by removing some edges from the clique. We show that adding in any missing edges will increase the principal ratio, and hence the extremal graph is exactly a kite graph.

2.2.2 Proof of main theorem

Let G be the graph with maximal principal ratio among all connected graphs on n vertices, and let k be the number of vertices in a shortest path between the vertices with smallest and largest eigenvalue entries. As above, let $x_1, \cdots, x_k$ be the vertices of the shortest path, where $\gamma(G) = \mathbf{v}_{x_k}/\mathbf{v}_{x_1}$. Let C be the set of vertices not on this shortest path, so $|C| = n-k$. Note that there is no graph with $n-k = 1$, as the endpoints of a path have the same principal eigenvector entry. Also $\lambda_1(G) \geq 2$, otherwise $P_{n-2} \cdot K_3$ would have larger principal ratio. Finally note that k is strictly larger than 1, otherwise $\mathbf{v}_{x_k} = \mathbf{v}_{x_1}$ and G would be regular.

Lemma 2.2.3. $\lambda_1(G) > n-k$.

Proof. Let H be the graph $P_k \cdot K_{n-k+1}$. It is straightforward to see that in H, the smallest entry of the principal eigenvector is the vertex of degree 1 and the largest is the vertex of degree $n-k+1$. Also note that in H, the vertices on the path P_k form a pendant path. By maximality we know that $\gamma(G) \geq \gamma(H)$. Combining this with lemma 2.2.1, we get

$$\frac{\sigma^k - \sigma^{-k}}{\sigma - \sigma^{-1}} \geq \gamma(G) \geq \gamma(H) = \frac{\sigma_H^k - \sigma_H^{-k}}{\sigma_H - \sigma_H^{-1}}$$

where $\sigma_H = \left(\lambda_1(H) + \sqrt{\lambda_1(H)^2 - 4}\right)/2$.
Now the function

$$f(x) = \frac{x^k - x^{-k}}{x - x^{-1}}$$

is increasing when $x \geq 1$. Hence we have $\sigma \geq \sigma_H$, and so $\lambda_1(G) \geq \lambda_1(H) > n-k$. $\square$

Lemma 2.2.4. *$x_1, x_2, \cdots, x_{k-2}$ are a pendant path in G, and x_k is connected to every vertex in G that is not on this path.*

Proof. By our choice of scaling, $\mathbf{v}_{x_k} = 1$. From lemma 2.2.3

$$n-k < \lambda_1(G) = \sum_{y \sim x_k} \mathbf{v}_y \leq |N(x_k)|.$$

Now $|N(x_k)|$ is an integer, so we have $|N(x_k)| \geq n-k+1$. Moreover because $x_1, x_2, \cdots, x_k$ is an induced path, we must have that $|N(x_k)| = n-k+1$ exactly, and hence the $N(x_k) = C \cup \{x_{k-1}\}$. It follows that $x_1, x_2, \cdots, x_{k-3}$ have no neighbors off the path, as otherwise there would be a shorter path between x_1 and x_k. $\square$

Lemma 2.2.5. *For the extremal graph G, we have $n-k = (1+o(1))\frac{n}{\log n}$.*

Proof. Let H be the graph $P_j \cdot K_{n-j+1}$ where $j = \left\lfloor n - \frac{n}{\log n} \right\rfloor$, and let G be the connected graph on n vertices with maximum principal ratio. Let $x_1, \cdots, x_k$ be a shortest path from x_1 to x_k where $\gamma(G) = \frac{\mathbf{v}_{x_k}}{\mathbf{v}_{x_1}}$. By lemma 2.2.4, we have

$$\lambda_1(G) \leq \Delta(G) \leq n-k+1.$$

By the eigenvector equation, this gives that

$$\gamma(G) \leq (n-k+1)^k \tag{2.1}$$

Now, lemma 2.2.1 gives that

$$\gamma(H) = \frac{\sigma_H^j - \sigma_H^{-j}}{\sigma_H - \sigma_H^{-1}},$$

where

$$\sigma(H) = \frac{\lambda_1(H) + \sqrt{\lambda_1(H)^2 - 4}}{2}.$$

Now, $s - 1 + \frac{1}{s(s-1)} < \lambda_1(P_r \cdot K_s) < s - 1 + \frac{1}{(s-1)^2}$, so we may choose n large enough that $\frac{n}{\log n} + 1 > \sigma_H - \sigma_H^{-1} > \frac{n}{\log n}$. By maximality of $\gamma(G)$, we have

$$(n-k+1)^k \geq \gamma(G) \geq \gamma(H) \geq \left(\frac{n}{\log n}\right)^{n - \frac{n}{\log n} - 2}.$$

Thus, $n - k = (1 + o(1))\frac{n}{\log n}$. □

For the remainder of this section we will explore the structure of G by showing that if certain edges are missing, adding them would increase the principal ratio, and so by maximality these edges must already be present in G. We have established that the vertices $x_1, x_2, \cdots, x_{k-2}$ are a pendant path, and so we have

$$\gamma(G) = \frac{\sigma^{k-2} - \sigma^{-k+2}}{\sigma - \sigma^{-1}} \frac{1}{\mathbf{v}_{x_{k-2}}} \tag{2.2}$$

We will not add any edges that affect this path, and so the above equality will remain true. The change in γ is then completely determined by the change in λ_1 and the change in $\mathbf{v}_{x_{k-2}}$. The next lemma gives conditions on these two parameters under which γ will increase or decrease.

Lemma 2.2.6. *Let $x_1, x_2, \cdots, x_{m-1}$ form a pendant path in G, where $n - m = (1 + o(1))n/\log(n)$. Let G_+ be a graph obtained from G by adding some edges from x_{m-1} to $V(G) \setminus \{x_1, \cdots, x_{m-1}\}$, where the addition of these edges does not affect which vertex has largest principal eigenvector entry. Let λ_1^+ be the largest eigenvalue of G_+ with leading eigenvector entry for vertex x denoted $\mathbf{v}_x^+$, also normalized to have maximum entry one. Define δ_1 and δ_2 such that $\lambda_1^+ = (1+\delta_1)\lambda_1$ and $\mathbf{v}_{x_{m-1}}^+ = (1+\delta_2)\mathbf{v}_{x_{m-1}}$. Then*

- $\gamma(G_+) > \gamma(G)$ *whenever* $\delta_1 > 4\delta_2/n$
- $\gamma(G_+) < \gamma(G)$ *whenever* $\delta_1 \exp(2\delta_1\lambda_1 \log n) < \delta_2/3n$.

Proof. We have

$$\sigma = \lambda_1 - \lambda_1^{-1} - \lambda_1^{-3} - 2\lambda_1^{-5} - \cdots - \frac{2}{2n-3}\binom{2n-2}{n}\lambda_1^{-(2n-1)} - \cdots$$

So

$$\lambda_1^+ - \lambda_1 < \sigma_+ - \sigma < \lambda_1^+ - \lambda_1 - 2((\lambda_1^+)^{-1} - \lambda_1^{-1})$$

when λ_1 is sufficiently large, which is guaranteed by lemma 2.2.5. Plugging in $\lambda_1^+ = (1+\delta_1)\lambda_1$, we get

$$\delta_1\lambda_1 < \sigma_+ - \sigma < \delta_1\lambda_1 + 2\lambda_1^{-1}(1-(1+\delta_1)^{-1}) < \delta_1\lambda_1 + \delta_1$$

In particular

$$(1+\delta_1/2)\sigma < \sigma_+ < (1+2\delta_1)\sigma$$

To prove part (i), we wish to find a lower bound in the change in the first factor of equation 2.2. Let

$$f(x) = \frac{x^{m-1} - x^{-m+1}}{x - x^{-1}}.$$

Then $2mx^{m-3} > f'(x) > (m-2)x^{m-3} - mx^{m-5}$, and using that $n - m \sim n/\log(n)$ and

$\sigma \sim \lambda_1$ which goes to infinity with n, we get $f'(x) \gtrsim (m-2)x^{m-3}$. By linearization and because $f(\sigma) \sim \sigma^{m-2}$, it follows that

$$\frac{\sigma_+^{m-1} - \sigma_+^{-m+1}}{\sigma_+ - \sigma_+^{-1}} \geq \left(1 + \frac{\delta_1(m-3)}{2}\right) \frac{\sigma^{m-1} - \sigma^{-m+1}}{\sigma - \sigma^{-1}}$$

Hence, if

$$\frac{\delta_1(m-3)}{2} > \delta_2$$

then $\gamma(G_+) > \gamma(G)$. In particular it is sufficient that $\delta_1 > 4\delta_2/n$.

To prove part (ii), recall from above that $f'(x) < 2mx^{m-3}$. Then, when $x = (1+o(1))(n/\log(n))$

$$\begin{aligned} f'(x+\varepsilon) &< 2m(x+\varepsilon)^{m-3} \\ &= 2mx^{m-3}\left(1+\frac{\varepsilon}{x}\right)^{m-3} \\ &\leq 2mx^{m-3}\exp\left(\frac{m\varepsilon}{x}\right) \\ &\leq 2nx^{m-3}\exp(2\log(n)\varepsilon) \end{aligned}$$

So for $0 < \varepsilon < \delta_1\lambda_1$, we have

$$f'(x+\varepsilon) < 2nx^{m-3}\exp(2\log(n)\delta_1\lambda_1)$$

Hence

$$\left(1 + 3n\exp(2\delta_1\lambda_1\log n)\delta_1\right)\frac{\sigma^{m-1} - \sigma^{-m+1}}{\sigma - \sigma^{-1}} > \frac{\sigma_+^{m-1} - \sigma_+^{-m+1}}{\sigma_+ - \sigma_+^{-1}}$$

$\square$

Lemma 2.2.7. *For every subset of U of $N(x_k)$, we have*

$$|U|-1<\sum_{y\in U}\mathbf{v}_y\leq |U|.$$

An immediate consequence is that there is at most one vertex in the neighborhood of x_k with eigenvector entry smaller than $1/2$.

Proof. The upper bound follows from $\mathbf{v}_y \leq 1$, and the lower bound from the inequalities

$$\sum_{y\in N(x_k)\setminus U}\mathbf{v}_y\leq |N(x_k)|-|U|$$

and

$$\sum_{y\in N(x_k)}\mathbf{v}_y=\lambda_1(G)>|N(x_k)|-1.$$

□

Lemma 2.2.8. *The vertex x_{k-2} has degree exactly 2 in G.*

Proof. Assume to the contrary. Let $U=N(x_{k-2})\cap N(x_k)$. Then $|U|\geq 2$, so by lemma 2.2.7 we have

$$\sum_{y\in U}\mathbf{v}_y>|U|-1\geq 1.$$

Now, by the same argument as the in the proof of lemma 2.2.1, we have that

$$\gamma(G)=\frac{\sigma^{k-1}-\sigma^{-k+1}}{\sigma-\sigma^{-1}}\left(\sum_{y\in U}\mathbf{v}_y\right)^{-1}$$

Let $H=P_{k-1}\cdot K_{n-k+2}$. Then by maximality of $\gamma(G)$ we have

$$\frac{\sigma^{k-1}-\sigma^{-k+1}}{\sigma-\sigma^{-1}}>\gamma(G)\geq\gamma(H)=\frac{\sigma_H^{k-1}-\sigma_H^{-k+1}}{\sigma_H-\sigma_H^{-1}}$$

So $\sigma > \sigma_H$, which means $\lambda_1(G) > \lambda_1(H) > n-k+1$. This means that $\Delta(G) > n-k+1$, but we have established that $\Delta(G) = n-k+1$. □

We now know that $x_1, x_2, \cdots, x_{k-1}$ is a pendant path in G, and so equation 2.2 becomes

$$\gamma(G) = \frac{\sigma^{k-1} - \sigma^{-k+1}}{\sigma - \sigma^{-1}} \frac{1}{\mathbf{v}_{x_{k-1}}} \tag{2.3}$$

Lemma 2.2.9. *The vertex x_{k-1} has degree less than $11|C|/\sqrt{\log n}$.*

Proof. Assume to the contrary, so throughout this proof we assume that the degree of x_{k-1} is at least $11|C|/\sqrt{\log n}$. Let G_+ the graph obtained form G with an additional edge from x_{k-1} to a vertex $z \in C$ with $\mathbf{v}_z \geq 1/2$. Let $\lambda_1^+ = \lambda_1(G_+)$ and let $\mathbf{v}_x^+$ be the principal eigenvector entry of vertex x in G_+, where this eigenvector is normalized to have $\mathbf{v}_{x_k}^+ = 1$.

Change in λ_1: By equation 1.2.2, we have $\lambda_1^+ - \lambda_1 \geq 2\frac{\mathbf{v}_{x_{k-1}}\mathbf{v}_z}{||\mathbf{v}||_2^2}$. A crude upper bound on $||\mathbf{v}||_2^2$ is

$$||\mathbf{v}||_2^2 \leq 1 + \sum_{y \sim x_k} \mathbf{v}_y + \frac{2}{\lambda_1} + \frac{4}{\lambda_1^2} + \cdots < 2\lambda_1$$

We also have that $\mathbf{v}_z \geq 1/2$ so

$$\lambda_1^+ \geq \left(1 + \frac{\mathbf{v}_{x_{k-1}}}{2\lambda_1^2}\right)\lambda_1.$$

Change in $\mathbf{v}_{x_{k-1}}$: Let $U = N(x_{k-1} \cap C)$. By the eigenvector equation we have

$$\begin{aligned}
\mathbf{v}_{x_{k-1}} &= \frac{1}{\lambda_1}\left(\mathbf{v}_{x_{k-2}} + \mathbf{v}_{x_k} + \sum_{y \in U} \mathbf{v}_y\right) \\
\mathbf{v}_{x_{k-1}}^+ &= \frac{1}{\lambda_1^+}\left(\mathbf{v}_{x_{k-2}}^+ + \mathbf{v}_{x_k}^+ + \mathbf{v}_z^+ + \sum_{y \in U} \mathbf{v}_y^+\right)
\end{aligned}$$

Subtracting these, and using that $\lambda_1 < \lambda_1^+$ and $\mathbf{v}_{x_k} = \mathbf{v}_{x_k}^+ = 1$, we get

$$\mathbf{v}_{x_{k-1}}^+ - \mathbf{v}_{x_{k-1}} \leq \frac{1}{\lambda_1}\left(\mathbf{v}_{x_{k-2}}^+ - \mathbf{v}_{x_{k-2}} + \mathbf{v}_z^+ + \sum_{y\in U} \mathbf{v}_y^+ - \mathbf{v}_y\right).$$

By lemma 2.2.7, we have $\sum_{y\in U} \mathbf{v}_y^+ - \mathbf{v}_y \leq 1$. We also have $\mathbf{v}_{x_{k-2}}^+ - \mathbf{v}_{x_{k-2}} < 1$ and $\mathbf{v}_z^+ \leq 1$. Hence $\mathbf{v}_{x_{k-1}}^+ - \mathbf{v}_{x_{k-1}} \leq 3/\lambda_1$, or

$$\mathbf{v}_{x_{k-1}}^+ \geq \left(1 + \frac{3}{\lambda_1 \mathbf{v}_{x_{k-1}}}\right)\mathbf{v}_{x_{k-1}}$$

We can only apply lemma 2.2.6 if $\mathbf{v}_{x_k}^+$ is the largest eigenvector entry in G_+. So we must consider two cases.

Case 1: If in G^+ the largest eigenvector entry is still attained by vertex $\mathbf{v}_{x_k}$, then we can apply lemma 2.2.6, and see that $\gamma(G^+) > \gamma(G)$ if

$$\frac{\mathbf{v}_{x_{k-1}}}{2\lambda_1^2} \geq \frac{12}{\lambda_1 \mathbf{v}_{x_{k-1}} n}$$

or equivalently

$$\mathbf{v}_{x_{k-1}}^2 \geq \frac{24\lambda_1}{n}.$$

We have that $\lambda_1 = (1+o(1))(n - n/\log(n))$, so it suffices for

$$\mathbf{v}_{x_{k-1}} \geq \frac{5}{\sqrt{\log n}}. \tag{2.4}$$

We know that

$$\mathbf{v}_{x_{k-1}} > \frac{|U|-1}{2\lambda_1}.$$

By assumption

$$|U| + 2 = N(x_{k-1}) \geq 11|C|/\sqrt{\log n}$$

Equation 2.4 follows from this, so $\gamma(G^+) > \gamma(G)$.

Case 2: Say the largest eigenvector entry of G^+ is no longer attained by vertex x_k. It is easy to see that the largest eigenvector entry is not attained by a vertex with degree less than or equal to 2, and comparing the neighborhood of any vertex in C with the neighborhood of x_k we can see that $\mathbf{v}_{x_k} \geq \mathbf{v}_y$ for all $y \in C$. So the largest eigenvector entry must be attained by $\mathbf{v}_{x_{k-1}}$. Then equation 2.3 no longer holds, instead we have

$$\gamma(G_+) = \frac{\sigma_+^{k-1} - \sigma_+^{-k+1}}{\sigma_+ - \sigma_+^{-1}}. \tag{2.5}$$

Recall that in lemma 2.2.6 we determined the change from $\gamma(G_+)$ to $\gamma(G)$ by considering $\lambda_1^+ - \lambda_1$ and $\mathbf{v}_{x_{k-1}}^+ - \mathbf{v}_{x_{k-1}}$. In this case, by (2.5), we must consider $\lambda_1^+ - \lambda_1$ and $1 - \mathbf{v}_{x_{k-1}}$. Now if $\mathbf{v}_{x_{k-1}}^+ > \mathbf{v}_{x_k}^+$, then vertex x_{k-1} in G is connected to all of C except perhaps a single vertex. Hence in G, the vertex x_{k-1} is connected to all of C except at most two vertices. This gives the bound

$$1 - \mathbf{v}_{x_{k-1}} \leq 3/\lambda_1$$

and so as in the previous case, $\gamma(G_+) > \gamma(G)$.

So in all cases, x_{k-1} is connected to all vertices in C that have eigenvector entry larger than $1/2$. If all vertices in C have eigenvector entry larger than $1/2$, then x_{k-1} is connected to all of C, and this implies that $\mathbf{v}_{x_{k-1}} > \mathbf{v}_{x_k}$, which is a contradiction. At most one vertex in C is smaller than $1/2$, and so there is a single vertex $z \in C$ with $\mathbf{v}_z < 1/2$. We will quickly check that adding the edge $\{x_{k-1}, z\}$ increases the principal ratio. As before let G_+ be the graph obtained by adding this edge. The largest eigenvector entry in G_+ is attained by x_{k-1}, as its neighborhood strictly contains the neighborhood of x_k. As above, adding the edge $\{z, x_k\}$ increases the spectral radius at least

$$\lambda_1^+ > \left(1 + \frac{\mathbf{v}_z}{2\lambda_1^2}\right)\lambda_1$$

and we have $1-\mathbf{v}_{x_{k-1}} < 1-\mathbf{v}_z/\lambda_1$. Applying lemma 2.2.6 we see that $\gamma(G_+) > \gamma(G)$, which is a contradiction. Finally we conclude that the degree of x_{k-1} must be smaller than $11|C|/\sqrt{\log n}$. □

We note that this lemma gives that $\mathbf{v}_{x_{k-1}} < 1/2$ which implies that any vertex in C has eigenvector entry larger than $1/2$.

Lemma 2.2.10. *The vertex x_{k-1} has degree exactly 2 in G. It follows that $\mathbf{v}_{x_{k-1}} < 2/\lambda_1$.*

Proof. Let $U = N(x_{k-1}) \cap C$, $c = |U|$. If $c = 0$ then we are done. Otherwise let G_- be the graph obtained from G by deleting these C edges. We will show that $\gamma(G_-) > \gamma(G)$.
(1) Change in λ_1: We have by equation 1.2.2,

$$\lambda_1 - \lambda_1^- \leq 2c\frac{\mathbf{v}_{x_{k-1}}}{||\mathbf{v}||_2^2}$$

By Cauchy–Schwarz,

$$||\mathbf{v}||_2^2 > \sum_{x\in N(x_k)} \mathbf{v}_x^2 \geq \frac{\left(\sum_{x\in N(x_k)} \mathbf{v}_x\right)^2}{|C|+1} \geq \frac{(n-k)^2}{n-k+1}$$

We also have

$$\mathbf{v}_{x_{k-1}} \leq \frac{c+2}{\lambda_1}$$

Combining these we get

$$\lambda_1 - \lambda_1^- < \frac{9c^2}{\lambda_1(n-k+1)} \Rightarrow \lambda_1 < \left(1+\frac{9c^2}{\lambda_1\lambda_1^-(n-k+1)}\right)\lambda_1^-$$

We have $\lambda_1\lambda_1^- > (n-k)^2$, so

$$\lambda_1 < \left(1+\frac{10c^2}{(n-k)^3}\right)\lambda_1^-$$

(2) Change in $\mathbf{v}_{x_{k-1}}$: At this point, we know that in G_- the vertices $x_1, \cdots, x_k$ form a pendant path, and so by the proof of lemma 2.2.1, we have $\mathbf{v}^-_{x_{k-1}} = (1+o(1))/\lambda_1$. By the eigenvector equation and using that the vertices in C have eigenvector entry at least $1/2$, we have $\mathbf{v}_{x_{k-1}} > (1+c/2)/\lambda_1$. So

$$\mathbf{v}_{x_{k-1}} - \mathbf{v}^-_{x_{k-1}} > \frac{1}{\lambda_1}\left(\frac{c}{2} + o(1)\right)$$

In particular,

$$\mathbf{v}_{x_{k-1}} > \left(1 + \frac{c}{3\mathbf{v}^-_{x_{k-1}}\lambda_1}\right)\mathbf{v}^-_{x_{k-1}}$$

Applying lemma 2.2.6, it suffices now to show that

$$\frac{10c^2}{(n-k)^3}\exp\left(2\frac{10c^2}{(n-k)^3}\lambda_1^- \log n\right) < \frac{c}{9\mathbf{v}^-_{x_{k-1}}\lambda_1 n}. \tag{2.6}$$

Now

$$\frac{10c^2}{(n-k)^3} < 10\frac{11^2}{\log(n)}\frac{|C|^2}{(n-k)^3} < \frac{11^3}{\log n}\frac{\log n}{n} = \frac{11^3}{n}.$$

Similarly $2\frac{10c^2}{(n-k)^3}\lambda_1^- \log n < 2\cdot 11^3$, so the lefthand side of equation 2.6 is smaller than C_0/n, where C_0 is an absolute constant. For the righthand side, recall that $\mathbf{v}^-_{x_{k-1}}\lambda_1 = 1+o(1)$, and also that

$$c > \frac{11}{\sqrt{\log n}}\left(\frac{n}{\log n} + o(1)\right) > \frac{10n}{\log^{3/2} n}.$$

So the righthand side is larger than $1/\log^{3/2} n$. Hence for large enough n, the righthand side is larger than the lefthand side.

□

We are now ready to prove the main theorem.

Theorem 1. *For sufficiently large n, the connected graph G on n vertices with largest* *principal ratio is a kite graph.*

Proof. It remains to show that C induces a clique. Assume it does not, and let H be the graph $P_k \cdot K_{n-k+1}$. We will show that $\gamma(H) > \gamma(G)$, and this contradiction tells us that C is a clique. As before, lemma 2.2.1 gives that

$$\gamma(H) = \frac{\sigma_H^k - \sigma_H^{-k}}{\sigma_H - \sigma_H^{-1}},$$

where

$$\sigma(H) = \frac{\lambda_1(H) - \sqrt{\lambda_1(H)^2 - 4}}{2}.$$

Since $x_1, \cdots x_k$ form a pendant path we also know that

$$\gamma(G) = \frac{\sigma^k - \sigma^{-k}}{\sigma - \sigma^{-1}}.$$

Now, $\lambda_1(H) > \lambda_1(G)$ because $E(G) \subsetneq E(H)$. Since the functions $g(x) = x + \sqrt{x^2 - 4}$ and $f(x) = (x^k - x^{-k})/(x - x^{-1})$ are increasing when $x \geq 1$, we have $\gamma(H) > \gamma(G)$.

□

2.3 Connected graphs of maximum irregularity

2.3.1 Structural lemmas

Throughout this section, let G be a graph on n vertices with spectral radius λ_1 and first eigenvector normalized so that $x = 1$. Throughout we will use $d = 2e(G)/n$ to denote the average degree. We will also assume that G is the connected graph on n vertices that maximizes $\lambda_1 - d$.

To show that G is a pineapple graph we first show that $\lambda_1 \sim \frac{n}{2}$ and $d \sim \frac{n}{4}$ (Lemma

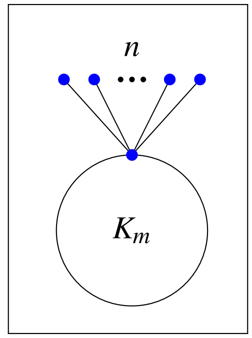

Figure 2.1: The pineapple graph, $PA(m,n)$.

2.3.1). Then we show that there exists a vertex with degree close to $\frac{n}{2}$ and eigenvector entry close to 1 (Lemma 2.3.3). We bootstrap this to show that there are many vertices of degree about $\frac{n}{2}$, that these vertices induce a clique, and further that most of the remaining vertices have degree 1 (Lemma 2.3.4 and Proposition 2.3.5). We complete the proof by showing that all vertices not in the clique have degree 1 and that they are all adjacent to the same vertex.

We remark that once we show that G is a pineapple graph, the small question remains of *which* pineapple graph maximizes $\lambda_1 - d$. Optimization of a cubic polynomial shows that G is a pineapple with clique size $\lceil \frac{n}{2} \rceil + 1$ (see [4], section 6).

Lemma 2.3.1. *We have* $\lambda_1(G) = \frac{n}{2} + c_1\sqrt{n}$ *and* $\frac{2e(G)}{n} = \frac{n}{4} + c_2\sqrt{n}$, *where* $|c_1|, |c_2| < 1$.

Proof. By eigenvalue interlacing, $\mathrm{PA}(p,q)$ has spectral radius at least $p-1$. Setting $H = \mathrm{PA}\left(\lceil \frac{n}{2} \rceil + 1, \lfloor \frac{n}{2} \rfloor - 1\right)$, we have

$$\lambda_1(H) - \frac{2e(H)}{n} \geq \frac{n}{4} - \frac{3}{2}.$$

On the other hand, an inequality of Hong [53] gives

$$\lambda_1^2 \leq 2e(G) - (n-1).$$

It follows that

$$d \geq \frac{\lambda_1^2}{n} + 1 - \frac{1}{n}. \tag{2.7}$$

Setting $\lambda_1 = pn$ and applying (2.7), we have $\lambda_1 - d \leq pn - p^2 n - 1 + \frac{1}{n}$. The right hand side of the inequality is maximized at $p = 1/2$, giving

$$\frac{n}{4} - \frac{3}{2} \leq \lambda_1 - d \leq \frac{n}{4} - 1 + \frac{1}{n}. \tag{2.8}$$

Next setting $\lambda_1 = \frac{n}{2} + c_1\sqrt{n}$, (2.7) gives

$$d \geq \frac{n}{4} + c_1\sqrt{n} + c_1^2 + 1 - \frac{1}{n},$$

whereas (2.8) implies

$$d \leq \lambda_1 - \frac{n}{4} + \frac{3}{2} = \frac{n}{4} + c_1\sqrt{n} + \frac{3}{2}. \tag{2.9}$$

Together, these imply $|c_1| < 1$ and prove both statements for n large enough. □

Lemma 2.3.2. *There exists a constant c_3 not depending on n such that*

$$0 \leq \frac{1}{|N(x)|} \sum_{y \sim x} d_y - \lambda_1 \mathbf{v}_y \leq c_3\sqrt{n}.$$

Proof. From the inequality of Hong,

$$\sum_{y \sim x} \lambda_1 \mathbf{v}_y = \lambda_1^2 \leq dn - (n-1).$$

Rearranging and applying Lemma 2.3.1, we have

$$0 \leq \sum_{y \sim x} (d_y - \lambda_1 \mathbf{v}_y) = O\left(n^{3/2}\right).$$

By equation (1.1) again, and because the first eigenvector is normalized with $\mathbf{v}_x = 1$, we have

$$\lambda_1 = \sum_{y \sim x} \mathbf{v}_y \le d_x,$$

giving $d_x = \Omega(n)$. Combining, we have

$$\frac{1}{|N(x)|} \sum_{y \sim x} (d_y - \lambda_1 \mathbf{v}_y) = O\left(\sqrt{n}\right),$$

where the implied constant is independent of n. □

Now we fix a constant $\varepsilon > 0$, whose exact value will be chosen later. The next lemma implies that close to half of the vertices of G have eigenvector entry close to 1 for n sufficiently large, depending on the chosen ε. We follow that with a proposition which outlines the approximate structure of G, and then finally use variational arguments to deduce that G is exactly a pineapple graph.

Lemma 2.3.3. *There exists a vertex $u \neq x$ with $\mathbf{v}_u > 1 - 2\varepsilon$ and $d_u - \lambda_1 \mathbf{v}_u = O(\sqrt{n})$. Moreover $d_u \geq (1/2 - 2\varepsilon)\, n$.*

Proof. We proceed by first showing a weaker result: that there is a vertex y with $\mathbf{v}_y > \frac{1}{2} - \varepsilon$ and $d_y - \lambda_1 \mathbf{v}_y = O(\sqrt{n})$, and additionally that $y \in N(x)$. We will then use this to obtain the required result.

Let $A := \{z \sim x : \mathbf{v}_z > \frac{1}{2} - \varepsilon\}$. By Lemma 2.3.1,

$$\lambda_1 = \frac{n}{2} + c_1 \sqrt{n},$$

where $|c_1| < 1$. Since $0 < \mathbf{v}_z \leq 1$ for all $z \sim x$, we see that $|A| \geq \delta_\varepsilon n$ where δ_ε is a positive constant that depends only on ε. Let $B = \{z \sim x : d_z - \lambda_1 \mathbf{v}_z > K\sqrt{n}\}$, where K is a fixed constant whose exact value will be chosen later. Now

$$\frac{1}{|N(x)|}\sum_{y\sim x}(d_y-\lambda_1\mathbf{v}_y)\geq\frac{1}{|N(x)|}\sum_{z\in B}(d_z-\lambda_1\mathbf{v}_z)\geq\frac{1}{n}|B|K\sqrt{n}.$$

By Lemma 2.3.2, $|B|\leq\frac{c_3}{K}n$. Therefore, for K large enough depending only on ε, we have $|A\cap B^c|>0$. This proves the existence of the vertex y, with the properties claimed at the beginning of the proof.

Next, we show that there exists a set $U\subset N(y)$ such that $|U|\geq\left(\frac{1}{4}-2\varepsilon\right)n$ and $\mathbf{v}_u\geq 1-2\varepsilon$ for all $u\in U$. By Lemma 2.3.1,

$$\left(\frac{n}{2}+c_1\sqrt{n}\right)\left(\frac{1}{2}-\varepsilon\right)\leq\lambda_1\mathbf{v}_y\leq d_y,$$

where $|c_1|<1$. So $d_y\geq\left(\frac{1}{4}-\varepsilon\right)n$ for n large enough. Now let $C=\{z\sim y:\mathbf{v}_z<1-2\varepsilon\}$. Then

$$K\sqrt{n}\geq d_y-\lambda_1\mathbf{v}_y=\sum_{z\sim y}(1-\mathbf{v}_z)\geq\sum_{z\in C}(1-\mathbf{v}_z)\geq 2|C|\varepsilon.$$

Therefore

$$|N(y)\setminus C|\geq\left(\frac{1}{4}-\varepsilon\right)n-\frac{K\sqrt{n}}{2\varepsilon}.$$

Setting $U=N(y)\setminus C$, we have $|U|>\left(\frac{1}{4}-2\varepsilon\right)n$ for n large enough.

Set $D=U\cap N(x)$. We will first find a lower bound on $|D|$. We have

$$\lambda_1^2\leq\sum_{y\sim x}d_y\leq 2m-\sum_{y\notin N(x)}d_y.$$

Rearranging this we get

$$d-\frac{\lambda_1^2}{n}\geq\frac{1}{n}\sum_{y\notin N(x)}d_y.$$

Now applying the bound on d from equation 2.9 and expression for λ_1 in Lemma 2.3.1

yields

$$\left(\frac{n}{4}+c_1\sqrt{n}+\frac{3}{2}\right)-\frac{\left(\frac{n}{2}+c_1\sqrt{n}\right)^2}{n}\geq\frac{1}{n}\sum_{y\notin N(x)}d_y,$$

which implies that

$$\frac{3}{2}n\geq\left(\frac{3}{2}-c_1^2\right)n\geq\sum_{y\notin N(x)}d_y\geq\sum_{y\in U\setminus N(x)}d_y\geq|U\setminus N(x)|(1-2\varepsilon)\lambda_1.$$

So

$$|U\setminus N(x)|\leq\frac{3}{2(1-2\varepsilon)}\frac{n}{\lambda_1}=\frac{3}{2(1-2\varepsilon)}\frac{1}{1/2+c_1n^{-1/2}}.$$

In particular, $|D|\geq(\frac{1}{4}-c'_\varepsilon)n$.

Now by the same argument used at the start of the proof to show the existence of the vertex y, we have some vertex $u\in D$ with $d_u-\lambda_1\mathbf{v}_u=O(\sqrt{n})$. Finally

$$d_u\geq\mathbf{v}_u\lambda_1\geq(1-2\varepsilon)(n/2+c_1\sqrt{n})\geq(1/2-2\varepsilon)n.$$

□

2.3.2 Alteration step

Lemma 2.3.4. *Let x,y be two vertices in G. If $\mathbf{v}_x\mathbf{v}_y>1/2+n^{-1/2}+5n^{-1}$, then x and y are adjacent. On the other hand, if $\mathbf{v}_x\mathbf{v}_y<1/2-3\varepsilon$ then x and y are not adjacent.*

Proof. We begin by bounding the dot product of the leading eigenvector $\mathbf{v}$ with itself. We will show that

$$\frac{n}{2}+\sqrt{n}+5\geq\mathbf{v}^t\mathbf{v}>\frac{n}{2}-2\varepsilon n-O(\sqrt{n}).\tag{2.10}$$

First, we show the lower bound. With u from the previous lemma, by Cauchy–Schwarz we have

$$\mathbf{v}^t\mathbf{v} \geq \sum_{z\sim u} \mathbf{v}_z^2 \geq \frac{1}{d_u}\left(\sum_{z\sim u} \mathbf{v}_z\right)^2 = \frac{(\lambda_1 \mathbf{v}_u)^2}{d_u}.$$

By Lemma 2.3.3, we then have

$$\mathbf{v}^t\mathbf{v} \geq \frac{(d_u - O(\sqrt{n}))^2}{d_u} \geq d_u - O(\sqrt{n}) > \frac{n}{2} - 2\varepsilon n - O(\sqrt{n}).$$

For the upper bound of inequality (2.10), first set $E = (N(x) \cup \{x\})^C$. Then

$$\mathbf{v}^t\mathbf{v} = \sum_{z\in V(G)} \mathbf{v}_z^2 \leq \sum_{z\in V(G)} \mathbf{v}_z \leq 1 + \sum_{z\in N(x)} \mathbf{v}_z + \sum_{z\in E} \mathbf{v}_z \leq 1 + \lambda_1 + \frac{1}{\lambda_1}\sum_{z\in E} d_z.$$

From the proof of Lemma 2.3.3 we have the bound

$$\sum_{z\in E} d_z \leq \frac{3}{2}n.$$

Hence

$$\mathbf{v}^t\mathbf{v} \leq 1 + \frac{n}{2} + c_1\sqrt{n} + \frac{3}{2}\cdot\frac{1}{1/2 + c_1 n^{-1/2}} \leq \frac{n}{2} + \sqrt{n} + 5.$$

This completes the proof of inequality (2.10).

Let λ_1^+ be the leading eigenvalue of the graph formed by adding the edge $\{x,y\}$ to G. Then by (1.2.2) we have

$$\lambda_1^+ - \lambda_1 \geq \frac{\mathbf{v}^t(A^+ - A)\mathbf{v}}{\mathbf{v}^t\mathbf{v}} \geq \frac{2\mathbf{v}_x\mathbf{v}_y}{\mathbf{v}^t\mathbf{v}} \geq \frac{2\mathbf{v}_x\mathbf{v}_y}{n/2 + \sqrt{n} + 5} = \frac{2\mathbf{v}_x\mathbf{v}_y}{n(1/2 + n^{-1/2} + 5n^{-1})}.$$

If $\mathbf{v}_x\mathbf{v}_y > 1/2 + n^{-1/2} + 5n^{-1}$, then

$$(\lambda_1^+ - d^+) - (\lambda - d) > \frac{2}{n} - \frac{2}{n} = 0.$$

Hence $\{x,y\}$ must already have been an edge, otherwise this would contradict the

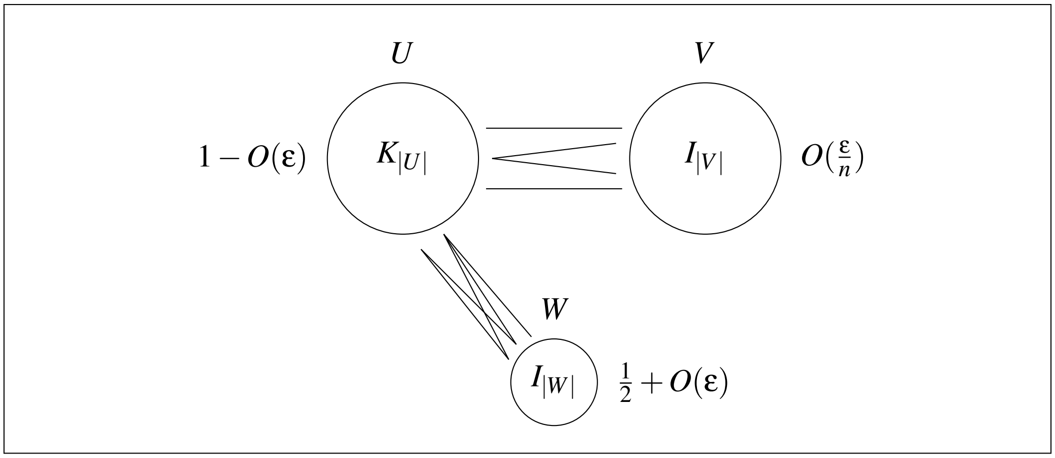

Figure 2.2: Structure of G in Proposition 2.3.5. The number beside each set indicates the values of eigenvector entries in the set. U is a clique and V, W are independent sets. Each vertex in V is adjacent to exactly one vertex in U, and each vertex in W is adjacent to multiple vertices in U.

maximality of G.

Similarly if λ_1^- is the leading eigenvalue of the graph obtained from G by deleting the edge $\{x,y\}$, then

$$\lambda_1-\lambda_1^- \le \frac{\mathbf{v}^t(A-A^-)\mathbf{v}}{\mathbf{v}^t\mathbf{v}} \le \frac{2\mathbf{v}_x\mathbf{v}_y}{n/2-2\varepsilon n-O(\sqrt{n})} \le \frac{2\mathbf{v}_x\mathbf{v}_y}{(1/2-3\varepsilon)n},$$

when n is large enough. Now if $\mathbf{v}_x\mathbf{v}_y < 1/2-3\varepsilon$, then

$$(\lambda_1-d)-(\lambda_1^- - d^-) < 0.$$

□

Proposition 2.3.5. *For n sufficiently large, we can partition the vertices of G into three sets U, V, W (see Figure 2.2) where*

(i) vertices in V have eigenvector entry smaller than $(2+\varepsilon)/n$ and have degree one,

(ii) vertices in U induce a clique, all have eigenvector entry larger than $1-20\varepsilon$, and $(1/2-3\varepsilon)n \le |U| \le (1/2+\varepsilon)n$,

(iii) vertices in W have eigenvector entry in the range $[1/2-4\varepsilon, 1/2+21\varepsilon]$ and are adjacent only to vertices in U.

Proof. By Lemma 2.3.4, any two vertices in G with eigenvector entry 1 are adjacent. Moreover, it is easy to see that every vertex in G is incident to at least one vertex with eigenvector entry 1: if not, for each vertex not incident to a vertex with eigenvector entry 1, delete one of its edges and add a new edge from that vertex to a vertex with eigenvector entry 1 (such as the vertex x). The resulting graph is connected, will have the same number of edges as the original graph, and will have strictly larger λ_1 (this can be seen by considering the Rayleigh quotient, as in the proof of Lemma 2.3.4). So by maximality of G, there are no such vertices. This implies that the set of edges that are incident to a vertex with eigenvector entry 1 spans the vertex set of G. In particular, if we remove any edge that is not incident to a vertex with eigenvector entry 1, we do not disconnect the graph. We will use this fact repeatedly in this proof.

(i) Let V consist of all vertices in G with eigenvector entry less than $1/2-4\varepsilon$. By Lemma 2.3.4, removing any edge incident to a vertex in V strictly increases $\lambda_1 - d$, so each vertex in V has degree one. By equation (1.1), the eigenvector entry of any such vertex is at most $1/\lambda_1 < (2+\varepsilon)/n$, when n is large enough.

(ii) From Lemma 2.3.3, we have a vertex u such that $d_u - \lambda_1 \mathbf{v}_u = O(\sqrt{n})$. Let X be the set of neighbors z of u such that $\mathbf{v}_z < 9/10$. Then we have

$$(1-9/10)|X| \le \sum_{y\sim u} 1-\mathbf{v}_y = d_u - \lambda_1 \mathbf{v}_u = O(\sqrt{n}).$$

Hence $|X| = O(\sqrt{n})$. Let U be all vertices in G with eigenvector entry at least

9/10. So, by Lemma 2.3.3

$$|U| \geq d_u - |X| \geq n/2 - 2\varepsilon n - O(\sqrt{n}).$$

For n large enough, we have $|U| \geq (1/2-3\varepsilon)n$. For sufficiently large n, by Lemma 2.3.4 these vertices are all adjacent to each other. For the upper bound on $|U|$ we use the expression for $e(G)$ in Lemma 2.3.1

$$|U|(|U|-1) \leq 2e(G) \leq \frac{n^2}{4} + c_2 n\sqrt{n},$$

which implies $|U| \leq (1/2+\varepsilon)n$ for large enough n.

Now take any vertex $y \in U$. If x is a vertex with largest eigenvector entry, then

$$\lambda_1 - \lambda_1 \mathbf{v}_y \leq \sum_{z \in N(x)\setminus N(y)} \mathbf{v}_z \leq \mathbf{v}_y + \sum_{z \in U^C} \mathbf{v}_z. \tag{2.11}$$

We have

$$\begin{aligned} \lambda_1 \sum_{z\in U^C} \mathbf{v}_z \leq \sum_{z \in U^C} d_z &\leq 2e(G) - 2|E(U,U)| \\ &\leq \frac{n^2}{4} + c_2 n\sqrt{n} - (1/2-3\varepsilon)(1/2-3\varepsilon-1/n)n^2 \\ &\leq 4\varepsilon n^2, \end{aligned}$$

for n sufficiently large, where we are using the expression for $e(G)$ given by Lemma 2.3.1. In particular,

$$\sum_{z \in U^C} \mathbf{v}_z \leq 9\varepsilon n.$$

Finally, by equation 2.11 we have

$$\mathbf{v}_y \geq 1 - \frac{1}{\lambda_1} \sum_{z \in U^C} \mathbf{v}_z - \frac{\mathbf{v}_y}{\lambda_1} \geq (1 - 20\varepsilon).$$

(iii) Let W consist of all remaining vertices of G. If a vertex has eigenvector entry smaller than $1/2 - 4\varepsilon$ then it is in V by construction. If a vertex $z \in W$ has eigenvector entry larger than $1/2 + 21\varepsilon$ then we have

$$(1/2 + 21\varepsilon)(1 - 20\varepsilon) > 1/2 + \varepsilon,$$

if $\varepsilon < 1/50$, say. So for sufficiently large n, by Lemma 2.3.4 we have that z is adjacent to every vertex in U. But by the proof of part (ii), this implies that $\mathbf{v}_z > 1 - 20\varepsilon$, which contradicts $z \in W$.

For $z \in W$ and any vertex $y \in U^C$, then $\mathbf{v}_y \mathbf{v}_z \leq (1/2+21\varepsilon)(1/2+21\varepsilon) < 1/4+22\varepsilon$ and so by Lemma 2.3.4 there is no edge between y and z in the maximal graph G.

□

2.3.3 The pineapple graph is extremal

Theorem 2.3.6. *For sufficiently large n, G is a pineapple graph.*

Proof. Take U, V, W as in the previous lemma. We begin by showing that the set W must be empty. Proceeding by contradiction, let z be in W. Furthermore let G^+ be the graph obtained by adding edges from z to every vertex in U. We will show that $\lambda_1(G^+) - d(G^+) > \lambda_1(G) - d(G)$, which contradicts the maximality of G.

Since the vertex z is adjacent only to vertices in U, and the fact that vertices in U

have eigenvector entry between $1-20\varepsilon$ and 1, equation (1.1) yields

$$\lambda_1(1/2-4\varepsilon) \leq \lambda_1 \mathbf{v}_z \leq d_z(G) \leq \frac{\lambda_1 \mathbf{v}_z}{1-20\varepsilon} = (1/2+O(\varepsilon))\lambda_1.$$

Using the expression for λ_1 in Lemma 2.3.1, for large enough n we have

$$(1-\varepsilon)\frac{n}{4} \leq d_z(G) \leq (1+\varepsilon)\frac{n}{4}.$$

So we can bound the change in the average degrees

$$d(G^+) - d(G) \leq \frac{2(|U|-(1-\varepsilon)n/4)}{n} < 1/2+3\varepsilon.$$

Next we find a lower bound on $\lambda_1(G^+)-\lambda_1(G)$. Let $\mathbf{w}$ be the vector that is equal to $\mathbf{v}$ on all vertices except z, and equal to 1 for z. Then,

$$\lambda_1(G^+) \geq \frac{\mathbf{w}^t A^+ \mathbf{w}}{\mathbf{w}^t \mathbf{w}}.$$

We first find a lower bound for the numerator (with abuse of big-O notation with inequalities)

$$\begin{aligned}
\mathbf{w}^t A^+ \mathbf{w} &\geq \mathbf{w}^t A \mathbf{w} + 2(|U| - d_z(G))(1-O(\varepsilon)) \geq \mathbf{w}^t A \mathbf{w} + (1/2 - O(\varepsilon))n \\
&\geq \mathbf{v}^t A \mathbf{v} + 2d_z(G)\,(1-\mathbf{v}_z)\,(1-20\varepsilon) + (1/2-O(\varepsilon))n \\
&\geq \mathbf{v}^t A \mathbf{v} + 2d_z(G)\,(1/2-31\varepsilon) + (1/2-O(\varepsilon))n \\
&\geq \mathbf{v}^t A \mathbf{v} + (3/4-O(\varepsilon))n.
\end{aligned}$$

Similarly, we find an upper bound for the denominator

$$\begin{aligned}\mathbf{w}^t\mathbf{w} &= \mathbf{v}^t\mathbf{v}+1-\mathbf{v}_z^2\\ &\leq \mathbf{v}^t\mathbf{v}+1-(1/2-4\varepsilon)^2\\ &\leq \mathbf{v}^t\mathbf{v}+3/4+4\varepsilon.\end{aligned}$$

Combining these, and using the bound on $\mathbf{v}^t\mathbf{v}$ from the proof of Lemma 2.3.4, we get

$$\begin{aligned}\lambda_1(G^+)-\lambda_1(G) &\geq \frac{\mathbf{w}^tA^+\mathbf{w}}{\mathbf{w}^t\mathbf{w}}-\frac{\mathbf{v}^tA\mathbf{v}}{\mathbf{v}^t\mathbf{v}}\\ &\geq \frac{\mathbf{v}^t\mathbf{v}(3/4-O(\varepsilon))n-\mathbf{v}^tA\mathbf{v}(3/4+4\varepsilon)}{\mathbf{v}^t\mathbf{v}(\mathbf{v}^t\mathbf{v}+3/4+4\varepsilon)}\\ &\geq \frac{(3/4-O(\varepsilon))n-(3/4+4\varepsilon)\lambda_1(G)}{\mathbf{v}^t\mathbf{v}+3/4+4\varepsilon}\\ &= 3/4+O(\varepsilon).\end{aligned}$$

Hence $\lambda_1(G^+)-\lambda_1(G) > d(G^+)-d(G)$, and by maximality of G we conclude that $W=\emptyset$.

At this point we know that G consists of a clique together with a set of pendant vertices V. All that remains is to show that all of the pendant vertices are incident to the same vertex in the clique. Let $V=\{v_1,v_2,\cdots,v_k\}$, and let u_i be the unique vertex in U that v_i is adjacent to. Let G^+ be the graph obtained from G by deleting the edges $\{v_i,u_i\}$ and adding the edges $\{v_i,x\}$, where x is a vertex with eigenvector entry 1. Now, $d(G^+)=d(G)$, and

$$\lambda_1(G^+)-\lambda_1(G)\geq \frac{\mathbf{v}^tA^+\mathbf{v}}{\mathbf{v}^t\mathbf{v}}-\frac{\mathbf{v}^tA\mathbf{v}}{\mathbf{v}^t\mathbf{v}},$$

with equality if and only if $\mathbf{v}$ is a leading eigenvector for A^+. We have

$$\frac{\mathbf{v}^tA^+\mathbf{v}}{\mathbf{v}^t\mathbf{v}}-\frac{\mathbf{v}^tA\mathbf{v}}{\mathbf{v}^t\mathbf{v}}=\frac{1}{\mathbf{v}^t\mathbf{v}}\left(\sum_{i=1}^{k}1-\mathbf{v}_{u_i}\right)\geq 0,$$

with equality if and only if $\mathbf{v}_{u_i} = 1$ for all $1 \leq i \leq k$. By maximality of G, we have equality in both of the above inequalities, and so $\mathbf{v}$ is a leading eigenvector for G^+, and every vertex in U incident to a vertex in V has eigenvector entry 1. G^+ is a pineapple graph, and it is easy to see that there is a single vertex in a pineapple graph with maximum eigenvector entry. It follows that the vertices in V are all adjacent to the same vertex in U, and hence G is a pineapple graph. □

This chapter is based on the papers "Three conjectures in extremal spectral graph theory", [51], to appear in *Journal of Combinatorial Theory, Series B*, and "Characterizing graphs of maximum principal ratio", submitted to *Electronic Journal of Linear Algebra* [50], both written jointly with Michael Tait. The dissertation author was the primary investigator and author of the paper.

Chapter 3

The spectral radius of outerplanar and planar graphs

3.1 Introduction

The study of spectral radius of planar graphs has a long history, dating back to at least Schwenk and Wilson [37]. This direction of research was further motivated by applications where the spectral radius is used as a measure of the connectivity of a network, in particular for planar networks in areas such as geography, see for example [8] and its references. In the field of geography, the spectral radius of the adjacency matrix was being used as a "summary measure of overall network connectivity" ([8]) of planar networks. To compare this statistic for two networks with different numbers of vertices, it is necessary to normalize by dividing out the maximum spectral radius of a planar graph on n vertices. To this end, Boots and Royle and independently Cao and Vince conjectured that the extremal graph is $P_2 + P_{n-2}$ [8], [11]. Several researchers have worked on this problem and successively improved upon the best theoretical upper bound, including [53], [11], [54], [30], [55], [22]. Other related problems have been considered, for example Dvořák and Mohar found an upper bound on the spectral radius of planar graphs with a given maximum degree [20]. Work has also been done maximizing the spectral radius of graphs on surfaces of higher genus [22, 54, 55]. We would also like to note that it is claimed in [22] that Guiduli and Hayes proved that the maximum spectral radius of a planar graph is attained by $P_2 + P_{n-2}$, for sufficiently large n. However, this preprint has never appeared, and the authors could not be reached for comment on it.

The outerplanar conjecture appeared in [17], where the authors mention that it is related to the study of various subfamilies of Hamiltonian graphs. Rowlinson [48] made partial progress on this conjecture, which was also worked on by Cao and Vince [11] and Zhou–Lin–Hu [57].

3.2 Outerplanar graphs of maximum spectral radius

Let G be a graph. As before, let the first eigenvector of the adjacency matrix of G be $\mathbf{v}$ normalized so that maximum entry is 1. For $v \in V(G)$ we will use v to mean a vertex or the eigenvector entry of that vertex, where it will be clear from context which meaning we are using. Let x be a vertex with maximum eigenvector entry, ie $x = 1$. Throughout let G be an outerplanar graph on n vertices with maximal adjacency spectral radius. λ_1 will refer to $\lambda_1(A(G))$.

Two consequences of G being outerplanar that we will use frequently are that G has at most $2n-3$ edges and G does not contain $K_{2,3}$ as a subgraph. An outline of our proof is as follows. We first show that there is a single vertex of large degree and that the remaining vertices have small eigenvector entry (Lemma 3.2.3). We use this to show that the vertex of large degree must be adjacent to every other vertex (Lemma 3.2.4). From here it is easy to prove that G must be $K_1 + P_{n-1}$.

We begin with an easy lemma that is clearly not optimal, but suffices for our

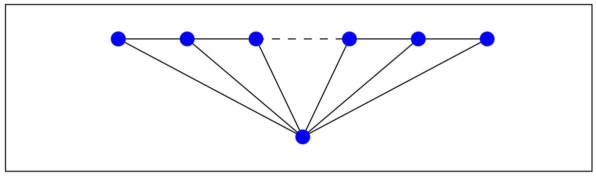

Figure 3.1: The graph $P_1 + P_{n-1}$.

needs.

Lemma 3.2.1. $\lambda_1 > \sqrt{n-1}$.

Proof. The star $K_{1,n-1}$ is outerplanar, and cannot be the maximal outerplanar graph with respect to spectral radius because it is a strict subgraph of other outerplanar graphs on the same vertex set. Hence, $\lambda_1(G) > \lambda_1(K_{1,n}) = \sqrt{n-1}$. □

Lemma 3.2.2. *For any vertex u, we have $d_u > \mathbf{v}_u n - 11\sqrt{n}$.*

Proof. Let A be the neighborhood of u, and let $B = V(G) \setminus (A \cup \{u\})$. We have

$$\lambda_1^2 \mathbf{v}_u = \sum_{y\sim u} \sum_{z\sim y} \mathbf{v}_z \leq d_u + \sum_{y\sim u} \sum_{z\in N(y)\cap A} \mathbf{v}_z + \sum_{y\sim u} \sum_{z\in N(y)\cap B} \mathbf{v}_z.$$

By outerplanarity, each vertex in A has at most two neighbors in A, otherwise G would contain a $K_{2,3}$. In particular,

$$\sum_{y\sim u} \sum_{z\in N(y)\cap A} \mathbf{v}_z \leq 2 \sum_{y\sim u} \mathbf{v}_y = 2\lambda_1 \mathbf{v}_u.$$

Similarly, each vertex in B has at most 2 neighbors in A. So

$$\sum_{y\sim u} \sum_{z\in N(y)\cap B} \mathbf{v}_z \leq 2 \sum_{z\in B} \mathbf{v}_z \leq \frac{2}{\lambda_1} \sum_{z\in B} d_z \leq \frac{4e(G)}{\lambda_1} \leq \frac{4(2n-3)}{\lambda_1},$$

as $e(G) \leq 2n-3$ by outerplanarity. So, using Lemma 3.2.1 we have

$$\sum_{y \sim u} \sum_{z \in N(y) \cap B} \mathbf{v}_z < 8\sqrt{n}.$$

Combining the above inequalities yields

$$\lambda_1^2 \mathbf{v}_u - 2\lambda_1 \mathbf{v}_u < d_u + 8\sqrt{n}.$$

Again using Lemma 3.2.1 we get

$$\mathbf{v}_u n - 11\sqrt{n} < (n-1-2\sqrt{n-1})\mathbf{v}_u - 8\sqrt{n} < d_u.$$

□

Lemma 3.2.3. *We have $d_x > n - 11\sqrt{n}$ and for every other vertex u, $\mathbf{v}_u < C_1/\sqrt{n}$ for some absolute constant C_1, for n sufficiently large.*

Proof. The bound on d_x follows immediately from the previous lemma and the normalization that $\mathbf{v}_x = 1$. Now consider any other vertex u. We know that G contains no $K_{2,3}$, so $d_u < 12\sqrt{n}$, otherwise u and x share $\sqrt{n}$ neighbors, which yields a $K_{2,3}$ if $n \geq 9$. So

$$12\sqrt{n} > d_u > \mathbf{v}_u n - 11\sqrt{n},$$

that is, $\mathbf{v}_u < 23/\sqrt{n}$. □

Lemma 3.2.4. *Let $B = V(G) \setminus (N(x) \cup \{x\})$. Then*

$$\sum_{z \in B} \mathbf{v}_z < C_2/\sqrt{n}$$

for some absolute constant C_2.

Proof. From the previous lemma, we have $|B| < 11\sqrt{n}$. Now

$$\sum_{z\in B} \mathbf{v}_z \leq \frac{1}{\lambda_1} \sum_{z\in B} \left(23/\sqrt{n}\right) d_z = \frac{23}{\lambda_1\sqrt{n}} \left(e(A,B) + 2e(B)\right).$$

Each vertex in B is adjacent to at most two vertices in A, so $e(A,B) \leq 2|B| < 22\sqrt{n}$. The graph induced on B is outerplanar, so $e(B) \leq 2|B| - 3 < 22\sqrt{n}$. Finally, using the fact that $\lambda_1 > \sqrt{n-1}$, we get the required result. □

Theorem 3.2.5. *For sufficiently large n, G is the graph $K_1 + P_{n-1}$, where + represents the graph join operation.*

Proof. First we show that the set B above is empty, i.e. x is adjacent to every other vertex. If not, let $y \in B$. Now y is adjacent to at most two vertices in A, and so by Lemma 3.2.3 and Lemma 3.2.4,

$$\sum_{z\sim y} \mathbf{v}_z < \sum_{z\in B} \mathbf{v}_z + 2C_1/\sqrt{n} < (C_2 + 2C_1)/\sqrt{n} < 1$$

when n is large enough. Let G^+ be the graph obtained from G by deleting all edges incident to y and replacing them by the single edge $\{x,y\}$. The resulting graph is outerplanar. Then, using the Rayleigh quotient,

$$\lambda_1(A^+) - \lambda_1(A) \geq \frac{\mathbf{v}^t (A^+ - A)\mathbf{v}}{\mathbf{v}^t\mathbf{v}} = \frac{2\mathbf{v}_y}{\mathbf{v}^t\mathbf{v}} \left(1 - \sum_{z\sim y} \mathbf{v}_z\right) > 0.$$

This contradicts the maximality of G. Hence B is empty.

Now x is adjacent to every other vertex in G. Hence every vertex other than x has degree less than or equal to 3. Moreover, the graph induced by $V(G)\setminus\{x\}$ cannot contain any cycles, as then G would not be outerplanar. It follows that G is a subgraph of $K_1 + P_{n-1}$, and maximality ensures that G must be equal to $K_1 + P_{n-1}$. □

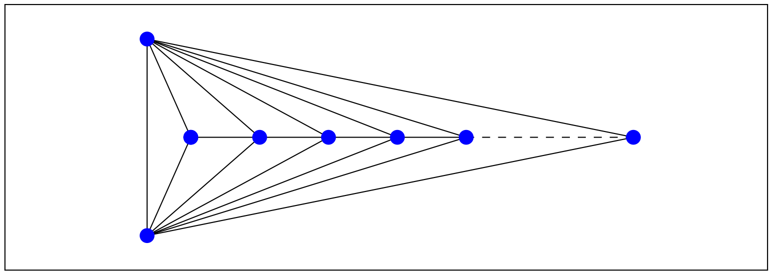

Figure 3.2: The graph $P_2 + P_{n-2}$.

3.3 Planar graphs of maximum spectral radius

3.3.1 Structural lemmas

As before, let G be a graph with first eigenvector normalized so that maximum entry is 1, and let x be a vertex with maximum eigenvector entry, ie $x = 1$. Let $m = |E(G)|$. For subsets $X, Y \subset V(G)$ we will write $E(X)$ to be the set of edges induced by X and $E(X,Y)$ to be the set of edges with one endpoint in X and one endpoint in Y. We will let $e(X,Y) = |E(X,Y)|$. We will often assume n is large enough without saying so explicitly. Throughout the section, let G be the planar graph on n vertices with maximum spectral radius, and let λ_1 denote this spectral radius.

We will use frequently that G has no $K_{3,3}$ as a subgraph, that $m \leq 3n-6$, and that any bipartite subgraph of G has at most $2n-4$ edges. The outline of our proof is as follows. We first show that G has two vertices that are adjacent to most of the rest of the graph (Lemmas 3.3.1–3.3.4). We then show that the two vertices of large degree are adjacent (Lemma 3.3.6), and that they are adjacent to every other vertex (Lemma 3.3.7). The proof of the theorem follows readily.

Lemma 3.3.1. $\sqrt{6n} > \lambda_1 > \sqrt{2n-4}$.

Proof. For the lower bound, first note that the graph $K_{2,n-2}$ is planar and is a strict subgraph of some other planar graphs on the same vertex set. Since G has maximum spectral radius among all planar graphs on n vertices,

$$\lambda_1 > \lambda_1(K_{2,n-2}) = \sqrt{2n-4}.$$

For the upper bound, since the sum of the squares of the eigenvalues equals twice the number of edges in G, which is at most $6n-12$ by planarity, we get that $\lambda_1 < \sqrt{6n-12} < \sqrt{6n}$. □

Next we partition the graph into vertices of small eigenvector entry and those with large eigenvector entry. Fix $\varepsilon > 0$, whose exact value will be chosen later. Let

$$L := \{\mathbf{v}_z \in V(G) : \mathbf{v}_z > \varepsilon\}$$

and $S = V(G) \setminus L$. For any vertex z, equation (1.1) gives $\mathbf{v}_z\sqrt{2n-4} < \mathbf{v}_z\lambda_1 \leq d_z$. Therefore,

$$2(3n-6) \geq \sum_{z\in V(G)} d_z \geq \sum_{z\in L} d_z \geq |L|\varepsilon\sqrt{2n-4},$$

yielding $|L| \leq \frac{3\sqrt{2n-4}}{\varepsilon}$. Since the subgraph of G consisting of edges with one endpoint in L and one endpoint in S is a bipartite planar graph, we have $e(S,L) \leq 2n-4$, and since the subgraphs induced by S and by L are each planar, we have $e(S) \leq 3n-6$ and $e(L) \leq \frac{9\sqrt{2n-4}}{\varepsilon}$.

Next we show that there are two vertices adjacent to most of S. The first step towards this is an upper bound on the sum of eigenvector entries in both L and S.

Lemma 3.3.2.

$$\sum_{z\in L} \mathbf{v}_z \leq \varepsilon\sqrt{2n-4} + \frac{18}{\varepsilon} \tag{3.1}$$

and

$$\sum_{z\in S} \mathbf{v}_z \leq (1+3\varepsilon)\sqrt{2n-4}. \tag{3.2}$$

Proof.

$$\begin{aligned}\sum_{z\in L}\lambda_1\mathbf{v}_z=\sum_{z\in L}\sum_{y\sim z}\mathbf{v}_y &= \sum_{z\in L}\left(\sum_{\substack{y\sim z\\ y\in S}}\mathbf{v}_y+\sum_{\substack{y\sim z\\ y\in L}}\mathbf{v}_y\right)\\ &\le \varepsilon e(S,L)+2e(L)\\ &\le \varepsilon(2n-4)+\frac{18\sqrt{2n-4}}{\varepsilon}.\end{aligned}$$

Dividing both sides by λ_1 and using Lemma 3.3.1 gives (3.1).

On the other hand,

$$\sum_{z\in S}\lambda_1\mathbf{v}_z=\sum_{z\in S}\sum_{y\sim z}\mathbf{v}_y\le 2\varepsilon e(S)+e(S,L)\le(6n-12)\varepsilon+(2n-4).$$

Dividing both sides by λ_1 and using Lemma 3.3.1 gives (3.2). □

Now, for $u\in L$ we have

$$\mathbf{v}_u\sqrt{2n-4}\le\lambda_1\mathbf{v}_u=\sum_{y\sim u}\mathbf{v}_y=\sum_{\substack{y\sim u\\ y\in L}}\mathbf{v}_y+\sum_{\substack{y\sim u\\ y\in S}}\mathbf{v}_y\le\sum_{y\in L}\mathbf{v}_y+\sum_{\substack{y\sim u\\ y\in S}}\mathbf{v}_y.$$

By (3.1), this gives

$$\sum_{\substack{y\sim u\\ y\in S}}\mathbf{v}_y\ge(\mathbf{v}_u-\varepsilon)\sqrt{2n-4}-\frac{18}{\varepsilon}. \tag{3.3}$$

The equations (3.2) and (3.3) imply that if $u\in L$ and $\mathbf{v}_u$ is close to 1, then the sum of the eigenvector entries of vertices in S not adjacent to u is small. The following lemma is used to show that u is adjacent to most vertices in S.

Lemma 3.3.3. *For all z we have $\mathbf{v}_z>\frac{1}{\sqrt{6n}}$.*

Proof. By way of contradiction assume $\mathbf{v}_z\le\frac{1}{\sqrt{6n}}<\frac{1}{\lambda_1}$. By equation (1.1) z cannot be adjacent to x, since x has eigenvector entry 1. Let H be the graph obtained from G

by removing all edges incident with z and making z adjacent to x. Using the Rayleigh quotient, we have $\lambda_1(H) > \lambda_1(G)$, a contradiction. □

Now letting $u = x$ and combining (3.3) and (3.2), we get

$$(1+3\varepsilon)\sqrt{2n-4} \geq \sum_{\substack{y\in S\\ y\not\sim x}} \mathbf{v}_y + \sum_{\substack{y\in S\\ y\sim x}} \mathbf{v}_y \geq \sum_{\substack{y\in S\\ y\not\sim x}} \mathbf{v}_y + (1-\varepsilon)\sqrt{2n-4} - \frac{18}{\varepsilon}.$$

Now applying Lemma 3.3.3 gives

$$|\{y \in S : y \not\sim x\}| \frac{1}{\sqrt{6n}} \leq 4\varepsilon\sqrt{2n-4} + \frac{18}{\varepsilon}.$$

For n large enough, we have $|\{y \in S : y \not\sim x\}| \leq 14\varepsilon n$. So x is adjacent to most of S. Our next goal is to show that there is another vertex in L that is adjacent to most of S.

Lemma 3.3.4. *There is a $w \in L$ with $w \neq x$ such that $\mathbf{v}_w > 1 - 24\varepsilon$ and $|\{y \in S : y \not\sim w\}| \leq 94\varepsilon n$.*

Proof. By equation (1.1), we see

$$\lambda_1^2 = \sum_{y\sim x}\sum_{z\sim y} \mathbf{v}_z \leq \left(\sum_{uv\in E(G)} \mathbf{v}_u + \mathbf{v}_v\right) - \sum_{y\sim x} \mathbf{v}_y = \left(\sum_{uv\in E(G)} \mathbf{v}_u + \mathbf{v}_v\right) - \lambda_1.$$

Rearranging and noting that $e(S) \leq 3n-6$ and $e(L) \leq \frac{9\sqrt{2n-4}}{\varepsilon}$ since S and L both induce planar subgraphs gives

$$\begin{aligned} 2n-4 \leq \lambda_1^2 + \lambda_1 \quad &\leq \quad \sum_{uv\in E(G)} \mathbf{v}_u + \mathbf{v}_v \\ &= \quad \left(\sum_{uv\in E(S,L)} \mathbf{v}_u + \mathbf{v}_v\right) + \left(\sum_{uv\in E(S)} \mathbf{v}_u + \mathbf{v}_v\right) + \left(\sum_{uv\in E(L)} \mathbf{v}_u + \mathbf{v}_v\right) \\ &\leq \quad \left(\sum_{uv\in E(S,L)} \mathbf{v}_u + \mathbf{v}_v\right) + \varepsilon(6n-12) + \frac{18\sqrt{2n-4}}{\varepsilon}. \end{aligned}$$

So for n large enough,

$$\begin{aligned}(2-7\varepsilon)n &\leq \sum_{uv\in E(S,L)} \mathbf{v}_u+\mathbf{v}_v \\ &= \left(\sum_{\substack{uv\in E(S,L)\\ u=x}} \mathbf{v}_u+\mathbf{v}_v\right)+\left(\sum_{\substack{uv\in E(S,L)\\ u\neq x}} \mathbf{v}_u+\mathbf{v}_v\right) \\ &\leq \varepsilon e(S,L)+d_x+\sum_{\substack{uv\in E(S,L)\\ u\neq x}} \mathbf{v}_u,\end{aligned}$$

giving

$$\sum_{\substack{uv\in E(S,L)\\ u\neq x}} \mathbf{v}_u \geq (1-9\varepsilon)n.$$

Now since $d_x \geq |S|-14\varepsilon n > (1-15\varepsilon)n$, and $e(S,L)<2n$, the number of terms in the left hand side of the sum is at most $(1+15\varepsilon)n$. By averaging, there is a $w\in L$ such that

$$\mathbf{v}_w \geq \frac{1-9\varepsilon}{1+15\varepsilon} > 1-24\varepsilon.$$

Applying (3.3) and (3.2) to this w gives

$$(1+3\varepsilon)\sqrt{2n-4} \geq \sum_{\substack{y\in S\\ y\not\sim w}} \mathbf{v}_y+\sum_{\substack{y\in S\\ y\sim w}} \mathbf{v}_y \geq \sum_{\substack{y\in S\\ y\not\sim w}} \mathbf{v}_y+(1-21\varepsilon)\sqrt{2n-4}+\frac{18}{\varepsilon},$$

and applying Lemma 3.3.3 gives that for n large enough

$$|\{y\in S: y\not\sim w\}| \leq 94\varepsilon n.$$

□

In the rest of the section, let w be the vertex from Lemma 3.3.4. So $\mathbf{v}_x = 1$

and $\mathbf{v}_w > 1-24\varepsilon$, and both are adjacent to most of S. Our next goal is to show that the remaining vertices are adjacent to both x and w. Let $B = N(x)\cap N(w)$ and $A = V(G)\setminus\{x\cup w\cup B\}$. We show that A is empty in two steps: first we show the eigenvector entries of vertices in A are as small as we need, which we then use to show that if there is a vertex in A then G is not extremal.

Lemma 3.3.5. *Let $v\in V(G)\setminus\{x,w\}$. Then $\mathbf{v}_v < \frac{1}{10}$.*

Proof. We first show that the sum over all eigenvector entries in A is small, and then we show that each eigenvector entry is small. Note that for each $v\in A$, v is adjacent to at most one of x and w, and is adjacent to at most 2 vertices in B (otherwise G would contain a $K_{3,3}$ and would not be planar). Thus

$$\lambda_1 \sum_{v\in A}\mathbf{v}_v \le \sum_{v\in A} d_v \le 3|A| + 2e(A) < 9|A|,$$

where the last inequality holds by $e(A) < 3|A|$ since A induces a planar graph. Now, since $|L| < \frac{3\sqrt{2n-4}}{\varepsilon} < \varepsilon n$ for n large enough, we have $|A| \le (14+94+1)\varepsilon n$ (by Lemma 3.3.4) . Therefore

$$\sum_{v\in A}\mathbf{v}_v \le \frac{9\cdot 109\cdot \varepsilon n}{\sqrt{2n-4}}.$$

Now any $v\in V(G)\setminus\{x,w\}$ is adjacent to at most 4 vertices in $B\cup\{x,w\}$, as otherwise we would have a $K_{3,3}$ as above. So we get

$$\lambda_1\mathbf{v}_v = \sum_{u\sim v}\mathbf{v}_u \le 4 + \sum_{\substack{u\sim v\\ u\in A}}\mathbf{v}_u \le 4 + \sum_{u\in A}\mathbf{v}_u \le C\varepsilon\sqrt{n},$$

where C is an absolute constant not depending on ε. Dividing both sides by λ_1 and choosing ε small enough yields the result. □

We use the fact that the eigenvector entries in A are small to show that if $v\in A$

(i.e. v is not adjacent to both x and w), then removing all edges from v and adding edges from it to x and w increases the spectral radius, showing that A must be empty. To do this, we must be able to add edges from a vertex to both x and w and have the resulting graph remain planar. This is accomplished by the following lemma.

Lemma 3.3.6. *If G is extremal, then $x \sim w$.*

Once $x \sim w$, one may add a new vertex adjacent to only x and w and the resulting graph remains planar.

Proof of Lemma 3.3.6. From above, we know that for any $\delta > 0$, we may choose ε small enough so that when n is sufficiently large we have $d_x > (1-\delta)n$ and $d_w > (1-\delta)n$. By maximality of G, we also know that G has precisely $3n-6$ edges, and by Euler's formula, any planar drawing of G has $2n-4$ faces, each of which is bordered by precisely three edges of G (because in a maximal planar graph, every face is a triangle).

Now we obtain a bound on the number of faces that x and w must be incident to. Let X be the set of edges incident to x. Each edge in G is incident to precisely two faces, and each face can be incident to at most two edges in X (again, since each face is a triangle by maximality). So x is incident to at least $|X| = d_x \geq (1-\delta)n$ faces. Similarly, w is incident to at least $(1-\delta)n$ faces.

Let F_1 be the set of faces that are incident to x, and then let F_2 be the set of faces that are not incident to x, but which share an edge with a face in F_1. Let $F = F_1 \cup F_2$. We have $|F_1| \geq (1-\delta)n$. Now each face in F_1 shares an edge with exactly three other faces: if two faces shared two edges, then since each face is a triangle both faces must be bounded by the same three edges; this cannot happen, except in the degenerate case when $n = 3$. At most two of these three faces are in F_1, and so $|F_2| \geq |F_1|/3 \geq (1-\delta)n/3$. Hence, $|F| \geq (1-\delta)4n/3$, and so the sum of the number of faces in F and the number of faces incident to w is larger than $2n-4$. In particular, there must be some face f that is both belongs to F and is incident to w.

Since $f \in F$, then either f is incident to x or f shares an edge with some face that is incident to x. If f is incident to both x and w, then x is adjacent to w and we are done. Otherwise, f shares an edge $\{y,z\}$ with a face f' that is incident to x. In this case, deleting the edge $\{y,z\}$ and inserting the edge $\{x,w\}$ yields a planar graph G'. By lemma 3.3.5, the product of the eigenvector entries of y and z is less than $1/100$, which is smaller than the product of the eigenvector entries of x and w. This implies that $\lambda_1(G') > \lambda_1(G)$, which is a contradiction. □

We now show that every vertex besides x and w is adjacent to both x and w.

Lemma 3.3.7. *A is empty.*

Proof. Assume that A is nonempty. A induces a planar graph, therefore if A is nonempty, then there is a $v \in A$ such that $|N(v) \cap A| < 6$. Further, v has at most 2 neighbors in B (otherwise G would contain a $K_{3,3}$. Recall that $\mathbf{v}$ is the principal eigenvector for the adjacency matrix of G. Let H be the graph with vertex set $V(G) \cup \{v'\} \setminus \{v\}$ and edge set $E(H) = E(G \setminus \{v\}) \cup \{v'x, v'w\}$. By Lemma 3.3.6, H is a planar graph. Then

$$
\begin{aligned}
\mathbf{v}^T\mathbf{v}\lambda_1(H) &\geq \mathbf{v}^T A(H)\mathbf{v} \\
&= \mathbf{v}^T A(G)\mathbf{v} - 2\sum_{z\sim v} \mathbf{v}_v\mathbf{v}_z + 2\mathbf{v}_v(\mathbf{v}_w + \mathbf{v}_x) \\
&\geq \mathbf{v}^T A(G)\mathbf{v} - 14 \cdot \mathbf{v}_v \cdot \frac{1}{10} - 2\sum_{\substack{z\sim v \\ z\in\{w,x\}}} \mathbf{v}_v\mathbf{v}_z + 2\mathbf{v}_v(\mathbf{v}_w + \mathbf{v}_x) && \text{(by Lemma 3.3.5)} \\
&\geq \mathbf{v}^T A(G)\mathbf{v} - \frac{14}{10}\mathbf{v}_v + 2\mathbf{v}_v\mathbf{v}_w && (|N(v) \cap \{x,w\}| \leq 1) \\
&> \mathbf{v}^T A(G)\mathbf{v} && (\text{as } \mathbf{v}_w > 7/10) \\
&= \mathbf{v}^T\mathbf{v}\lambda_1(G).
\end{aligned}
$$

So $\lambda_1(H) > \lambda_1(G)$ and H is planar, i.e. G is not extremal, a contradiction. □

We now have that if G is extremal, then $K_2 + I_{n-2}$, the join of an edge and an independent set of size $n-2$, is a subgraph of G. Finishing the proof is straightforward.

3.3.2 Proof of main theorem

Theorem 3.3.8. *For $n \geq N_0$, the unique planar graph on n vertices with maximum spectral radius is $K_2 + P_{n-2}$.*

Proof. By Lemmas 3.3.6 and 3.3.7, x and w have degree $n-1$. We now look at the set $B = V(G) \setminus \{x, w\}$. For $v \in B$, we have $|N(v) \cap B| \leq 2$, otherwise G contains a copy of $K_{3,3}$. Therefore, the graph induced by B is a disjoint union of paths, cycles, and isolated vertices. However, if there is some cycle C in the graph induced by B, then $C \cup \{x, w\}$ is a subdivision of K_5. So the graph induced by B is a disjoint union of paths and isolated vertices. However, if B does not induce a path on $n-2$ vertices, then G is a strict subgraph of $K_2 + P_{n-2}$, and we would have $\lambda_1(G) < \lambda_1(K_2 + P_{n-2})$. Since G is extremal, B must induce P_{n-2} and so $G = K_2 + P_{n-2}$. □

This chapter is based on part of the paper “Three conjectures in extremal spectral graph theory”, [51], to appear in *Journal of Combinatorial Theory, Series B*, written jointly with Michael Tait. The dissertation author was the primary investigator and author of the paper.

Chapter 4

The spectral gap of reversal graphs

4.1 Introduction

Consider a permutation τ in the symmetric group S_n, written in word notation $(\tau_1, \tau_2, \cdots, \tau_n)$, where we denote $\tau(i) = \tau_i$. A *substring* is a subsequence of τ, $(\tau_i, \tau_{i+1}, \ldots, \tau_j)$, for some $1 \leq i < j \leq n$, and *reversing* this substring yields $(\tau_j, \tau_{j-1}, \ldots, \tau_i)$. A *substring reversal* of τ is any permutation obtained from τ by reversing a substring in τ. Substring reversal is a well-studied operation on permutations, and often appears in metrics on permutations, edit distances and permutation statistics. There are numerous applications involving many variations of substring reversal, such as genome arrangements and sequencing (see [5], [32], [39]).

The *reversal graph* R_n is the graph whose vertex set is the permutation group S_n, where two vertices are adjacent if they are substring reversals of each other. Thus, R_n has $n!$ vertices and is regular with degree $\binom{n}{2}$. Many properties of the reversal graph R_n have long been studied. One interesting problem is to determine the minimum number of substring reversals needed to transform one given permutation in S_n to another, which is equivalent to finding a shortest path in R_n. The smallest number of reversals required to turn any permutation into any other is exactly the diameter of R_n, and it was shown in [5] that the diameter of the reversal graph is exactly $n-1$. The connectivity and hamiltonicity of R_n were investigated in [41]. There are still many questions concerning R_n that remain unresolved. In this section, we examine the eigenvalues of R_n, and determine the second largest eigenvalue of the adjacency matrix of R_n. Note that the second largest adjacency eigenvalue of a regular graph is intimately related to the rate of convergence for random walks on a graph. We use methods from graph coverings to determine the second largest eigenvalue of R_n, although our techniques cannot be used to determine the whole spectrum of R_n.

An intriguing variation of substring reversal is *prefix reversal* (or *pancake flipping*) where only substrings of the form $(\tau_1, \ldots, \tau_j)$ are allowed to be reversed. The *prefix reversal graph*, or the *pancake graph*, $\mathcal{P}_n$ is a special subgraph of R_n. $\mathcal{P}_n$ also has vertex set S_n but the edge set is restricted. In $\mathcal{P}_n$, the neighbors of τ are the permutations of the form

$$(\tau_k, \tau_{k-1}, \cdots, \tau_1, \tau_{k+1}, \cdots, \tau_n)$$

for $1 < k \leq n$. In contrast to the reversal graph where the exact value of the diameter is known, the problem of determining the diameter of the pancake graph has a long history and still remains open. This problem was first posed by Jacob Goodman, under the pseudonym Harry Dweighter, as a Monthly problem in 1975 [21]. The current best upper bound is $f(n) \leq \frac{18}{11}n$, due to Chitturi et al. [13], improving on a previous bound of $\frac{5}{3}n$ given by Gates and Papadimitriou [27] in 1979. The best lower bound is $f(n) \geq 15 \left\lfloor \frac{n}{14} \right\rceil$, which is due to Heydari and Sudborough [34]. Recently it was shown that the problem of determining the exact minimum number of flips to transform one permutation τ_1 into another permutation τ_2, for two given permutations τ_1 and τ_2, is NP–hard [10]. In [12], it was determined that the spectral gap of $\mathcal{P}_n$ is one, answering a question posed in [31]. We will determine the spectral gaps for a family of graphs which contains certain Cayley graphs including $\mathcal{P}_n$, giving an alternative proof in that case. We then use the spectral gap of $\mathcal{P}_n$, together with a decomposition of R_n into P_n and copies of R_{n-1}, to determine the second largest eigenvalue of R_n.

Theorem 4.1.1. *If λ_1, λ_2 are the two largest eigenvalues of the adjacency matrix of R_n, then*

$$\lambda_1 = \binom{n}{2}, \text{ and } \lambda_2 = \binom{n}{2} - n.$$

We will consider a family of graphs that generalizes the pancake graph, and show that for every graph in this family the spectral gap is one.

Theorem 4.1.2. *Let $\mathcal{F}_n$ be the set of all graphs whose vertex set is the symmetric group S_n, and where for each vertex τ and each $2 \leq i \leq n$, τ is adjacent to exactly one vertex of the form*

$$(\tau_i, \alpha_2, \alpha_3, \cdots, \alpha_{i-1}, \tau_1, \tau_{i+1}, \cdots, \tau_n).$$

That is, the first and ith entries are swapped, and the entries in between are possibly rearranged. Then for any graph $G \in \mathcal{F}_n$, the two largest eigenvalues of the adjacency matrix of G are $n-1$ and $n-2$. In particular, the adjacency spectral gap of G is 1.

The graphs R_n and $\mathcal{P}_n$, as well as many of the graphs in $\mathcal{F}_n$, are Cayley graphs of the symmetric group S_n. Indeed, Cayley graphs of the symmetric group have been the subject of extensive study, with particular interest in their spectral gap. In [42], Lubotzky posed the problem of finding a family of k-regular Cayley graphs of S_n with spectral gap bounded away from zero; an explicit construction of such a family was found in [38]. For many particular Cayley graphs of S_n, the spectral gap has been computed [26, 24, 12], and the case when S consists of transpositions is particularly well-studied. Of particular relevance here, the Cayley graph with generating set

$$S = \{(1\ k) : 2 \leq k \leq n\}$$

belongs to the family $\mathcal{F}_n$, and the spectral gap was determined to be 1 in [24].

The remainder of the paper is organized as follows. In Section 2 we review the necessary background and establish notation. In Section 3 we recall the notions of graph coverings and projections, which we will use frequently in our proofs. In Section 4 we introduce a graph which is a projection of every graph in the family $\mathcal{F}_n$, which provides a lower bound of one on the spectral gap of every graph in this family. We establish the corresponding upper bound in Section 5. In Section 6 we prove Theorem 4.1.1 and further investigate the spectrum of R_n. We conclude with some problems and remarks.

Before proceeding to define the graph spectra of interest here, we note that the definitions of eigenvalues and eigenvectors are much simpler and cleaner for regular graphs than those of weighted irregular graphs. Although the graphs R_n and the graphs in $\mathcal{F}_n$, are regular, we will consider various associated graphs which are irregular and weighted in order to determine the spectral gap that we need. Furthermore, we remark that the spectral gap of the adjacency matrix of a weighted or unweighted graph often depends on a few of the largest degrees and therefore the spectral gap of the adjacency matrix can *not* be used to determine the rate of convergence for random walks on irregular graphs. Instead it is more appropriate to study the combinatorial Laplacian and normalized Laplacian. In this section, we consider general weighted graphs and define the eigenvalues of the normalized Laplacian, which will be important when we define graph covers. For undefined terminology, the reader is referred to [15].

Let G denote a weighted undirected graph with edge weight $w_{u,v} = w_{v,u}$. The adjacency matrix of G, denoted by A_G, has entries $A_G(u,v) = w_{u,v}$ for vertices u and v. For any vertex $v \in V(G)$, the set of vertices adjacent to v is denoted by $N(v)$. The degree d_v of a vertex v is defined to be

$$d_v = \sum_u w_{u,v}.$$

We will only consider weighted graphs without isolated vertices, i.e., $d_v > 0$ for all v. Let

D_G be the diagonal degree matrix whose ith diagonal entry is equal to the degree of the ith vertex. Then the combinatorial Laplacian of G is $L_G = D_G - A_G$, and the normalized Laplacian is $\mathcal{L}_G = D_G^{-1/2} L_G D_G^{-1/2}$. For a d-regular graph, we have $\mathcal{L}_G = 1 - \frac{1}{d}A_G$. The eigenvalues of the normalized Laplacian $\mathcal{L}_G$ are denoted by $0 = \mu_0 \leq \mu_1 \leq \ldots \leq \mu_{n-1}$ where n is the number of vertices in G. μ_1 is called the spectral gap of the normalized Laplacian, and the rate of convergence of random walks on G with transition probability matrix $P = D_G^{-1} A_G$ is exactly μ_1^{-1} (see [15]). We will denote the eigenvalues of the adjacency matrix of G by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, and $\lambda_1 - \lambda_2$ is the spectral gap of the adjacency matrix. For a regular graph of degree d, $\lambda_1 = d$ and $\lambda_2 = d(1-\mu_1)$.

Let ϕ_i denote the orthonormal eigenvector associated with μ_i. It can easily be shown that $\phi_0 = D_G^{1/2}/\sqrt{\mathrm{vol}(G)}$ where $\mathrm{vol}(G) = \sum_v d_v$. Instead of dealing with eigenvectors ϕ_i of $\mathcal{L}_G$, it is often convenient to consider the corresponding *harmonic eigenfunction* defined by $f_i = D_G^{-1/2}\phi_i$ which satisfies

$$\mu_i f_i(u) d_u = \sum_v w_{u,v}(f(u) - f(v))$$

for all vertices u. Note that for regular graphs, harmonic eigenfunctions are exactly eigenfunctions. Moreover, for regular graphs the eigenfunctions of $\mathcal{L}, L$ and A are the same, and the corresponding spectra are translations of each other.

We will frequently deal with permutations, so we establish the notation that we will use. The symmetric group is denoted as S_n throughout. Every permutation will be given in *word notation*, that is, as a list of numbers $(\tau_1, \tau_2, \cdots, \tau_n)$, which indicates that permutation τ maps i to τ_i. We will sometimes refer to the value τ_i as the ith *entry* or *position* of the permutation τ. When we write the product of two permutations, such as $\pi\sigma$, we take this to mean: first apply permutation σ, then apply permutation π.

As discussed in Section 1, R_n and many of the graphs in the family $\mathcal{F}_n$ are Cayley graphs. We briefly recall the definition here. Let H be a finite group, and S a subset of H. We say that S is a symmetric set if whenever $s \in S$, we also have $s^{-1} \in S$. Given a symmetric set S that generates the group H, the right-Cayley graph $\mathrm{Cay}_R(H,S)$ is the graph with vertex set equal to H, and edges of the form $\{x, xs\}$ for all $x \in H, s \in S$. This is an undirected $|S|$-regular graph. A left-Cayley graph is defined similarly, with edges of the form $\{x, sx\}$. For example, let S be the set of permutations corresponding to substring reversals. That is, S consists of the permutations obtained from taking the identity permutation $(1,2,3,\cdots,n)$ and reversing a substring. Then $R_n = \mathrm{Cay}_R(S_n, S)$.

In proving Theorem 4.1.2 and Theorem 4.1.1, we will rely heavily on graph coverings, an idea developed in [14]. A short overview is presented here. Let G and $\tilde{G}$ be two weighted graphs. Then $\tilde{G}$ is a *covering* of G if there is a surjection $\pi : V(\tilde{G}) \to V(G)$ satisfying the following two properties:

(1) For $x, y \in V(\tilde{G})$, where $\pi(x) = \pi(y)$, and for any $v \in V(G)$

$$\sum_{z \in \pi^{-1}(v)} w(z,x) = \sum_{z \in \pi^{-1}(v)} w(z,y).$$

(2) There is a fixed $m \in \mathbb{R}^+ \cup \{\infty\}$, the *index* of π, such that for all $u, v \in V(G)$

$$\sum_{\substack{x \in \pi^{-1}(u) \\ y \in \pi^{-1}(v)}} w(x,y) = m w(u,v). \tag{4.1}$$

As π is a surjection, it can alternatively be viewed as a partition of the vertices of $V(\tilde{G})$ into $|V(G)|$ sets. With this interpretation, the above definition can be seen as a generalization of an *equitable partition*; see, for example, [28]. We say that G is a *projection* of $\tilde{G}$ via the mapping π if $\tilde{G}$ is a covering of G under π.

The virtue of a graph covering is that there is a strong correspondence between the eigenvalues of a covering graph and the eigenvalues of the projection. This correspondence is the content of the following theorem, which is proved in [14].

Theorem 4.1.3. (Covering-Correspondence)
Let $G, \tilde{G}$ be two weighted undirected graphs, and $\pi : V(\tilde{G}) \to V(G)$ be a covering map. For any function $f : V(\tilde{G}) \to \mathbb{C}$, define $p_f : V(G) \to \mathbb{C}$ by

$$p_f(v) = \sum_{x \in \pi^{-1}(v)} \frac{f(x) d_x}{d_v}.$$

For any function $f : V(G) \to \mathbb{C}$, define the lift of f, $l_f : V(\tilde{G}) \to \mathbb{C}$ by

$$l_f(x) = f(u), \text{ where } \pi(x) = u.$$

(i) If μ is an eigenvalue of G with harmonic eigenfunction f, then μ is an eigenvalue of $\tilde{G}$ with harmonic eigenfunction l_f.

(ii) If μ is an eigenvalue of $\tilde{G}$ with harmonic eigenfunction f, then if $p_f \neq 0$, μ is an eigenvalue of G with harmonic eigenfunction p_f.

We will use this theorem in the form of the following corollary.

Corollary 4.1.4. *Let G be a graph with cover $\tilde{G}$, under covering map π, where $\tilde{G}$ is a regular graph. Then the eigenvalues of the normalized Laplacian of G are eigenvalues of the normalized Laplacian of $\tilde{G}$. For any eigenvalue μ of the normalized Laplacian of $\tilde{G}$ that is not an eigenvalue of G, the corresponding eigenfunction f satisfies*

$$\sum_{x \in \pi^{-1}(u)} f(x) = 0 \tag{4.2}$$

for all $u \in V(G)$.

Furthermore, if G, $\tilde{G}$ are both regular graphs with the same degree d, then this holds for their adjacency matrices as well.

Proof. It follows directly from Theorem 4.1.3 that if μ is an eigenvalue of the normalized Laplacian of G, then it is an eigenvalue of $\tilde{G}$. Now let μ be an eigenvalue of $\tilde{G}$ with eigenfunction f, where μ is not an eigenvalue of G. By regularity of $\tilde{G}$, f is also a harmonic eigenfunction, and by part (ii) of Theorem 4.1.3 it must be the case that $p_f = 0$. Hence, for all $u \in V(G)$,

$$0 = p_f(u) = \frac{1}{d_u} \sum_{x \in \pi^{-1}(u)} f(x) d_x.$$

By regularity, d_x is constant, and so dividing by a constant gives equation 4.2.

If G, $\tilde{G}$ are both d-regular graphs, then their adjacency eigenvalues satisfy $\lambda_i = d(1 - \mu_{i-1})$, and the corresponding eigenfunctions are the same. It follows that adjacency eigenvalues of G are also adjacency eigenvalues of $\tilde{G}$, and for any other adjacency eigenvalue of $\tilde{G}$ the corresponding eigenfunction satisfies equation 4.2. □

Example. Let G be the Petersen graph. We compute the eigenvalues of G by finding a graph G' for which G is a cover. Define G' to be the weighted graph with vertex set $\{v_1, v_2, v_3\}$, and edges and edge weights as shown in Figure 4.1. The adjacency matrix and normalized Laplacian of G' are

$$A_{G'} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 2 \\ 0 & 2 & 4 \end{bmatrix}, \mathcal{L}_{G'} = \begin{bmatrix} 1 & -\frac{1}{\sqrt{3}} & 0 \\ -\frac{1}{\sqrt{3}} & 1 & -\frac{\sqrt{2}}{3} \\ 0 & -\frac{\sqrt{2}}{3} & \frac{1}{3} \end{bmatrix}$$

Now fix any vertex $x \in V(G)$, and define a map $\pi : V(G) \to V(G')$ by

$$\pi(y) = \begin{cases} v_1 & y = x \\ v_2 & y \sim x \\ v_3 & \text{otherwise} \end{cases}$$

It is easy to check that π satisfies the definition of a graph covering (with index $m = 3$), and so the eigenvalues of $\mathcal{L}_{G'}$, which are $0, \frac{2}{3}, \frac{5}{3}$, are eigenvalues of $\mathcal{L}_G$. Furthermore these must be the only eigenvalues of $\mathcal{L}_G$. Otherwise, let f be a harmonic eigenfunction corresponding to some other eigenvalue. By vertex transitivity of G, we can assume $f(x) \neq 0$. By the covering-correspondence theorem, since f does not correspond to an eigenvalue of G' we have that $p_f = 0$. Hence

$$0 = p_f(v_1) = \sum_{y \in \pi^{-1}(v_1)} f(y) \frac{d_y}{d_{v_1}} = f(x) d_x$$

since by construction of π, x is the only vertex mapped to v_1. It follows that $f(x) = 0$ which is a contradiction, and this shows that all of the eigenvalues of $\mathcal{L}_G$ are eigenvalues of $\mathcal{L}_{G'}$.

(a) Petersen graph G (b) Graph G'

Figure 4.1: The Petersen graph G and a three vertex weighted graph which it covers. In the covering map, vertices in G are sent to the vertex with same color in G'.

4.2 Spectral gap of graphs in $\mathcal{F}_n$

4.2.1 A projection of graphs in $\mathcal{F}_n$

We begin by constructing a weighted graph G_n on three vertices, which is a projection of every graph in $\mathcal{F}_n$. Then we compute the eigenvalues of G_n, and by Corollary 4.1.4, these will be eigenvalues of every graph in $\mathcal{F}_n$. Let F be a graph in $\mathcal{F}_n$, and let G_n be the weighted graph with vertices $\{v_1, v_2, v_3\}$, with edge weights $w(v_1, v_1) = n-2$, $w(v_1, v_2) = 1$, $w(v_2, v_3) = n-2$, $w(v_3, v_3) = (n-2)^2$, and all other edge weights zero. To construct the covering map $\pi : V(F) \to V(G_n)$, we just need to specify the sets $U_1 = \pi^{-1}(v_1), U_2 = \pi^{-1}(v_2), U_3 = \pi^{-1}(v_3)$:

$$\begin{aligned} U_1 = \pi^{-1}(v_1) &= \{\tau \in S_n : \tau_n = n\} \\ U_2 = \pi^{-1}(v_2) &= \{\tau \in S_n : \tau_1 = n\} \\ U_3 = \pi^{-1}(v_3) &= \{\tau \in S_n : \tau_1 \neq n, \tau_n \neq n\} \end{aligned}$$

In order to verify that this is a covering, we need to check the two properties:

(1) We need to show that any two vertices in the same preimage set U_i have the same number of neighbors in each preimage set U_j. For example, take $\tau \in U_3$, so $\tau_k = n$ for some $1 < k < n$. By definition of $\mathcal{F}_n$, if σ is adjacent to τ then either $\sigma_n = \tau_n$ or $\sigma_n = \tau_1$. In particular, $\sigma_n \neq n$, so τ is not adjacent to any vertex in U_1. There is exactly one neighbor of τ with $\sigma_1 = n$, and so τ is adjacent to exactly one vertex in U_1. The remaining $n-2$ neighbors of τ are in U_3. As required, the number of neighbors in each preimage set did not depend on the choice of $\tau \in U_3$. The cases that $\tau \in U_1$ and $\tau \in U_2$ are similar.

(2) We need to verify equation 4.1 for each pair chosen from the preimage sets

U_1, U_2, U_3. For this covering, we have $m = (n-1)!$. Firstly, U_1 and U_1:

$$\sum_{\substack{x \in U_1 \\ y \in U_1}} w(x,y) = \sum_{x \in U_1} (n-2)$$

since each element of U_1 is adjacent to exactly $n-2$ elements in U_1. So

$$\sum_{\substack{x \in U_1 \\ y \in U_1}} w(x,y) = |U_1|(n-2) = (n-1)!w(v_1, v_1)$$

as required. The pairs U_1, U_2 and U_2, U_3 are similarly verified.

For the pair U_1 and U_3, since there are no edges between these sets and since $w(v_1, v_3) = 0$, we are done. Similarly for the pair U_2 and U_2. And finally, the pair U_3, U_3:

$$\sum_{\substack{x \in U_3 \\ y \in U_3}} w(x,y) = \sum_{x \in U_3} (n-2) = |U_3|(n-2)$$

Now $|U_3| = n! - |U_1| - |U_2| = (n-2)(n-1)!$, so we get

$$\sum_{\substack{x \in U_3 \\ y \in U_3}} w(x,y) = (n-1)!w(v_3, v_3)$$

as required.

Now that we have a covering, we evaluate the eigenvalues of the projection G_n.

Lemma 4.2.1. *The eigenvalues of the normalized Laplacian of G_n are*

$0, \frac{1}{n-1}, \frac{n}{n-1}$.

Proof. The normalized Laplacian of G_n is

$$\begin{bmatrix} \frac{1}{n-1} & -\frac{1}{n-1} & 0 \\ -\frac{1}{n-1} & 1 & -\frac{\sqrt{n-2}}{n-1} \\ 0 & -\frac{\sqrt{n-2}}{n-1} & \frac{1}{n-1} \end{bmatrix}$$

The result follows from a simple computation. □

Corollary 4.2.2. *For any $G \in \mathcal{F}_n$, the adjacency matrix A_G has eigenvalues $n-1$, $n-2$ and -1. For $1 \leq i \leq n$ define*

$$\begin{aligned} X(i) &= \{\tau \in S_n : \tau_n = i\} \\ Y(i) &= \{\tau \in S_n : \tau_1 = i\} \\ Z(i) &= \{\tau \in S_n : \tau_1 \neq i, \tau_n \neq i\} \end{aligned}$$

Then any eigenfunction corresponding to any other eigenvalue than those listed above must sum to zero on each of $X(i)$, $Y(i)$ and $Z(i)$, for any $i \in \{1, 2, \cdots, n\}$.

Proof. When defining the covering mapping π to G_n, for a permutation τ the vertex it was mapped to was determined by the position of n in τ. Observe that we can replace n with any index i, $1 \leq i \leq n$, and we still have a covering, in this case with preimage sets $X(i), Y(i), Z(i)$.

Now take an eigenfunction of G which corresponds to an eigenfunction other than $n-1$, $n-2$, or -1. G is regular, so this eigenfunction is also an eigenfunction of the normalized Laplacian of G, corresponding to an eigenvalue other than 0, $1/(n-1)$ or $n/(n-1)$. It follows from Corollary 4.1.4 and the previous lemma that the eigenfunction must sum to zero over the preimage sets of the covering, which are $X(i)$, $Y(i)$ and $Z(i)$. □

4.2.2 The spectral gap is 1

Recall that $\mathcal{F}_n$ is the family of graphs whose vertex set is S_n and where for each vertex τ,

$$\tau = (\tau_1, \tau_2, \cdots, \tau_n),$$

and each $2 \leq i \leq n$, τ is adjacent to exactly one vertex of the form

$$(\tau_i, \alpha_2, \alpha_3, \cdots, \alpha_{i-1}, \tau_1, \tau_{i+1}, \cdots, \tau_n).$$

Each graph in $\mathcal{F}_n$ is an $(n-1)$-regular graph. The prefix reversal graph $\mathcal{P}_n$ is in $\mathcal{F}_n$, as well as the right-Cayley graph generated by the transpositions $(1\ k)$, where $2 \leq k \leq n$.

In order to compute the spectral gap of graphs in $\mathcal{F}_n$, we proceed by induction, so first we compute the spectrum of graphs in $\mathcal{F}_3$ to establish our base case.

Lemma 4.2.3. $\mathcal{F}_3 = \{C_6\}$. *In particular, the adjacency spectral gap of every graph in* $\mathcal{F}_3$ *is one.*

Proof. Let $G \in \mathcal{F}_3$. Then G is a 2-regular graph on $3! = 6$ vertices. From the definition of $\mathcal{F}_3$, it is easy to verify that G is connected, and so $G = C_6$. The first two adjacency eigenvalues of C_6 are 2 and 1. □

We can now prove the theorem on the spectral gap of $\mathcal{F}_n$, as stated in the Section 1.

Proof of Theorem 4.1.2. We proceed by induction, so assume that the adjacency spectral gap of any graph in $\mathcal{F}_{n-1}$ is 1. The base case is established by Lemma 4.2.3. By $(n-2)$-regularity of graphs in $\mathcal{F}_{n-1}$, it follows from the inductive assumption that the second largest eigenvalue of any graph in $\mathcal{F}_{n-1}$ is $n-3$.

Let G be a graph in $\mathcal{F}_n$. Pick any eigenvector f coming from an eigenvalue λ that is not $n-1$, $n-2$ or -1. Our goal is to show that $\lambda < n-2$. Recall that $X(i)$ consists of the permutations whose last entry is i, $Y(i)$ consists of the permutations whose first entry is i and $Z(i)$ consists of all other permutations. For any i, from Corollary 4.2.2 we get a projection of G with preimage sets $X(i), Y(i), Z(i)$. The set $X(i)$ induces a graph in $\mathcal{F}_{n-1}$, and the set $Y(i)$ induces an independent set (since every two adjacent permutations have different first entries). Furthermore the edges between $X(i)$ and $Y(i)$ form a matching. Our proof strategy is the following: we will get an expression for λ involving the values of f on the set $X(i)$ and the set $Y(i)$. We can control the contribution from $X(i)$ using the inductive assumption, and then we show that we can choose i so that the contribution from $Y(i)$ is small enough to yield the stated result.

Claim: We can fix an i such that

$$\sum_{x \in X(i)} f(x)^2 \geq \sum_{y \in Y(i)} f(y)^2 \tag{4.3}$$

and

$$\sum_{x \in X(i)} f(x)^2 > 0.$$

Proof of claim: Notice that the sets $X(1), X(2), \cdots, X(n)$ partition the vertex set of G (ie. partitioning the permutations based on the last entry). Similarly, the sets $Y(1), Y(2), \cdots, Y(n)$ partition the vertex set of G. Hence

$$\sum_{j=1}^{n} \sum_{x \in X(j)} f(x)^2 = \sum_{j=1}^{n} \sum_{y \in Y(j)} f(y)^2 > 0.$$

In particular, there exists an index i such that

$$\sum_{x \in X(i)} f(x)^2 \geq \sum_{y \in Y(i)} f(y)^2.$$

Let I denote the set of indices i satisfying the above inequality. Then there exists some i

in I satisfying

$$\sum_{x \in X(i)} f(x)^2 > 0$$

since $f \neq 0$. This proves the claim.

Consider an arbitrary vertex $x \in X(i)$. Then by definition of $X(i)$, x is a permutation with $x(n) = i$. x has $n-1$ neighbors in G, $n-2$ of these neighbors are in $X(i)$ and one of its neighbors is in $Y(i)$. Let c_x be the unique neighbor of x in $Y(i)$. As noted above, the induced subgraph on $X(i)$ is in $\mathcal{F}_{n-1}$. By the eigenvalue-eigenvector equation, we have

$$\lambda f(x) = f(c_x) + \sum_{y \in N(x) \cap X(i)} f(y).$$

Multiplying both sides by $f(x)$, and summing over $x \in X(i)$ yields

$$\lambda \sum_{x \in X(i)} f(x)^2 = \sum_{x \in X(i)} f(x) f(c_x) + \sum_{x \in X(i)} \sum_{y \in N(x) \cap X(i)} f(x) f(y).$$

Dividing across by the sum on the left-hand side (which is non-zero by our claim above) gives

$$\lambda = \frac{\sum_{x \in X(i)} f(x) f(c_x)}{\sum_{x \in X(i)} f(x)^2} + \frac{\sum_{x \in X(i)} \sum_{y \in N(x) \cap X(i)} f(x) f(y)}{\sum_{x \in X(i)} f(x)^2}. \tag{4.4}$$

We will now find upper bounds for each of the two terms on the right-hand side.

Let G' be the induced subgraph on $X(i)$, which is a graph in $\mathcal{F}_{n-1}$, and let $g = f|_{X(i)}$. Since $\sum_{x \in X(i)} f(x) = 0$, we have that $g \perp \mathbf{1}$, where $\mathbf{1}$ is the constant vector with entries 1, which is the eigenvector associated with λ_1. Now we can bound the second term in equation 4.4 by $n-3$:

$$\begin{aligned}
\frac{\sum_{x\in X(i)} \sum_{y\in N(x)\cap X(i)} f(x)f(y)}{\sum_{x\in X(i)} f(x)^2} &= \frac{g^T A_{G'} g}{g^T g} \\
&\leq \max_{h\perp \mathbf{1}} \frac{h^T A_{G'} h}{h^T h} \\
&= \lambda_2(G') \\
&= n-3.
\end{aligned}$$

The edges between $X(i)$ and $Y(i)$ are a matching. So as x ranges over the vertices of $X(i)$, c_x ranges over the vertices of $Y(i)$. By Cauchy–Schwarz,

$$\begin{aligned}
\sum_{x\in X(i)} f(x)f(c_x) &\leq \sqrt{\sum_{x\in X(i)} f(x)^2 \sum_{x\in X(i)} f(c_x)^2} \\
&= \sqrt{\sum_{x\in X(i)} f(x)^2 \sum_{y\in Y(i)} f(y)^2}
\end{aligned}$$

So

$$\frac{\sum_{x\in X(i)} f(x)f(c_x)}{\sum_{x\in X(i)} f(x)^2} \leq \sqrt{\frac{\sum_{y\in Y(i)} f(y)^2}{\sum_{x\in X(i)} f(x)^2}} \leq 1$$

where the last inequality follows from equation 4.3.

Applying these two bounds in equation 4.4 gives

$$\lambda \leq n-3+1 = n-2.$$

This shows that there is no eigenvalue of G strictly between $n-2$ and $n-1$, so we conclude that $\lambda_2(G) = n-2$. □

As a brief application of Theorem 4.1.2, we can establish bounds on the edge expansion of every graph in $G \in \mathcal{F}_n$. Recall that the edge expansion of a d-regular graph G, h_G, is defined as

$$h_G = \min_{S \subset V(G)} \frac{|E(S,\bar{S})|}{\min(|S|,|\bar{S}|) \cdot d}.$$

If S is the set of permutations whose last entry is n, then $|S| = |E(S,\bar{S})| = (n-1)!$, which gives the upper bound $h_G \leq 1/(n-1)$. To obtain a lower bound, we can use an inequality from [15], $h_G \geq \mu_1/2$. Combining these two inequalities gives the bounds

$$\frac{1}{2(n-1)} \leq h_G \leq \frac{1}{n-1}.$$

4.3 The reversal graph

4.3.1 A graph projection of the reversal graph

The graph R_n is a Cayley graph of S_n that does not belong to the family $\mathcal{F}_n$ but is closely related. For any $1 \leq i < j \leq n$, let $r_{i,j}$ denote the bijection on S_n defined by

$$r_{i,j}(\tau) = (\tau_1, \tau_2, \cdots, \tau_{i-1}, \tau_j, \tau_{j-1}, \cdots \tau_{i+1}, \tau_i, \tau_{j+1}, \cdots, \tau_n)$$

That is, it reverses the subsequence from indices i to j, inclusive. Then two permutations σ and τ are adjacent in R_n iff $\tau = r_{i,j}(\sigma)$ for some $i < j$. We will first show that R_n has many integer eigenvalues. We remark that the spectrum of R_n is not generally integer-valued, despite the presence of many integer eigenvalues. A plot of the 7! eigenvalues of R_7 is given in Figure 4.2. We will first prove the following useful fact.

Lemma 4.3.1. *Let X be the symmetric $n \times n$ matrix with entries*

$$X_{i,j} = min\{i, j, n+1-i, n+1-j\}$$

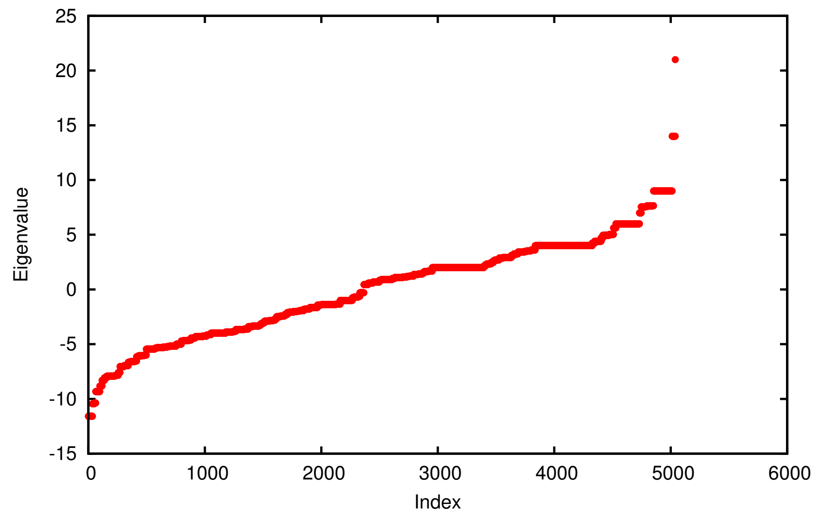

Figure 4.2: The adjacency eigenvalues of the reversal graph, R_7, plotted in increasing order.

For a given real number x, let D be the unique diagonal matrix such that every row of $D+X$ sums to x. Then the eigenvalues of $D+X$ are

$$\lambda_k = x - \left\lfloor \frac{k}{2} \right\rfloor n + 2\binom{\lfloor \frac{k}{2} \rfloor}{2}, 1 \leq k \leq n.$$

In particular, $\lambda_1 = x$, $\lambda_2 = x - n$.

Example: For $n = 5$ and $x = 12$ we get

$$D+X = \begin{pmatrix} 7 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 7 \end{pmatrix} + \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 & 1 \\ 1 & 2 & 3 & 2 & 1 \\ 1 & 2 & 2 & 2 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

which has eigenvalues $12, 7, 7, 4, 4$.

Proof. We proceed by induction. For the case $n = 1$, the result is immediate. When

$n = 2$, we have

$$D + X = \begin{pmatrix} x-1 & 1 \\ 1 & x-1 \end{pmatrix}$$

which has eigenvalues x and $x-2$, as required.

Now fix n and assume the result holds for all smaller dimensions. Since $D+X$ is a symmetric matrix with constant row sums, the leading eigenvector of $D+X$ is the all-ones vector $\mathbf{1}$, with corresponding eigenvalue x. All other eigenvectors are orthogonal to $\mathbf{1}$. It follows that if $Y = D + X - \mathbf{1}\mathbf{1}^T$, then $D+X$ and Y have the same eigenvectors. Moreover, the spectrum of Y, counting multiplicity, is exactly the spectrum of $D+X$ with x replaced by $x-n$.

The only non-zero entry in the top row of Y is the top-left entry, which is $x-n$. The only non-zero entry in the bottom row of Y is the bottom-right entry which is also $x-n$. Denote the characteristic polynomial of a matrix A by $p_A(\lambda)$. Expanding the determinant of $Y - \lambda I$ along the top row and then along the bottom row, we obtain that

$$p_Y(\lambda) = (\lambda - x + n)^2 p_{Y'}(\lambda)$$

where Y' is the $(n-2)\times(n-2)$ principal submatrix of Y, obtained by deleting the first and last rows and columns. In particular, the spectrum of Y consists of $x-n$ with multiplicity two, and the spectrum of Y'. Hence, from the relationship between the spectrum of $D+X$ and the spectrum of Y discussed above, we have that the eigenvalues of $D+X$ are exactly the eigenvalues of Y', together with x and $x-n$.

Observe that Y' satisfies the conditions of the theorem, with row sum equal to

$x-n$. By induction, we have that the eigenvalues of Y' are (for $1 \leq k \leq n-2$):

$$\begin{aligned} \lambda_k(Y') &= (x-n) - \left\lfloor \frac{k}{2} \right\rfloor (n-2) + 2\binom{\lfloor \frac{k}{2} \rfloor}{2} \\ &= x - \left\lfloor \frac{k+2}{2} \right\rfloor n + 2\binom{\lfloor \frac{k+2}{2} \rfloor}{2}. \end{aligned}$$

Combining these $n-2$ eigenvalues with x and $x-n$ yields exactly the claimed spectrum for $D+X$. □

Lemma 4.3.2. *The spectrum of the adjacency matrix of the reversal graph, A_{R_n}, contains the eigenvalues*

$$\lambda_k = \binom{n}{2} - \left\lfloor \frac{k}{2} \right\rfloor n + 2\binom{\lfloor \frac{k}{2} \rfloor}{2}, 1 \leq k \leq n.$$

In particular, $\binom{n}{2}$ and $\binom{n}{2} - n$ are eigenvalues, and so the spectral gap is at most n.

Proof. We begin by constructing a projection of the graph R_n. Let G be the graph with vertices $v_1, v_2, \cdots, v_n$ corresponding to the adjacency matrix $A_G = D+X$, where vertex v_i corresponds to row and column i, and $D+X$ is as in the previous lemma, with row sum $\binom{n}{2}$. Let $U(i)$ be the set of all permutations τ such that $\tau_i = n$. The sets $U(i)$, for $1 \leq i \leq n$, partition $V(R_n)$, so we can define a map $\pi : V(R_n) \to V(G)$ by setting $\pi(x) = v_i$ whenever $x \in U(i)$. It suffices to show that this is a covering map, then the result will follow from the previous lemma.

To show that π satisfies the first property of a graph cover, we need that for all indices i, j, any two vertices in $U(i)$ have the same number of neighbors in $U(j)$. This follows from the fact that there are a fixed number of reversals that map entry i to entry j.

For the second property, take two preimage sets $U(i)$, $U(j)$, and τ_0 some permutation in $U(j)$. It is easily checked that by construction of the weighted graph G, we have

$$w(v_i, v_j) = |N(\tau_0) \cap U(i)|.$$

Then

$$\begin{aligned}\sum_{\sigma\in U(i)}\sum_{\tau\in U(j)} w(\sigma,\tau) &= \sum_{\sigma\in U(i)} |U(j)|w(\sigma,\tau_0)\\ &= (n-1)!\,|N(\tau_0)\cap U(i)|\\ &= (n-1)!w(v_i,v_j)\end{aligned}$$

where the first equality follows from property (i). Hence π is a covering with $m=(n-1)!$.

□

4.3.2 The spectral gap of the reversal graph

We are finally ready to prove the main theorem determining the spectral gap of R_n.

Proof of Theorem 4.1.1: The value of λ_1 is $\binom{n}{2}$ since R_n is regular of degree $\binom{n}{2}$. From the previous lemma we have that

$$\lambda_2 \geq \binom{n}{2} - n$$

so it suffices to prove that

$$\lambda_2 \leq \binom{n}{2} - n.$$

We follow a similar approach to the proof of Theorem 4.1.2.

We proceed by induction. For the base case, consider $n=2$. Then R_2 is K_2, with eigenvalues $1,-1$. Now assume for any $m<n$, we have

$$\lambda_2(A_{R_m}) = \binom{m}{2} - m.$$

For any $1 \leq i \leq n$, we define the sets

$$U_i(j) = \left\{\tau \in S_n : \tau_j = i\right\}.$$

As in the proof of Lemma 4.3.2, for any fixed i the sets $U_i(j)$, $1 \leq j \leq n$ are the preimages of a covering map of R_n, and the two largest eigenvalues of the projection are $\binom{n}{2}$ and $\binom{n}{2} - n$. It follows from Corollary 4.1.4 that if A_{R_n} has an eigenvalue λ strictly between $\binom{n}{2}$ and $\binom{n}{2} - n$ then the corresponding eigenvector must sum to zero on $U_i(j)$ for all i, j. Let λ be such an eigenvalue, with eigenvector f.

Let $E_1 = \{\{\sigma, \tau\} \in E(R_n) : \sigma_1 \neq \tau_1\}$, that is, the set of edges arising from substring reversals that include the first entry of the permutation. Observe that the edge set E_1 is exactly the set of edges of the prefix reversal graph $\mathcal{P}_n$. Let R' be the graph obtained by removing all edges in E_1 from R_n. Then R' consists of n connected components, $U_1(1), U_2(1), \cdots, U_n(1)$. Each of these connected components is isomorphic to R_{n-1}.

We have, by the Rayleigh quotient

$$\begin{aligned}
\lambda &= \frac{2\sum_{\{x,y\}\in E(R_n)} f(x)f(y)}{\sum_{x\in R_n} f(x)^2} \\
&= \frac{2\sum_{\{x,y\}\in E_1} f(x)f(y)}{\sum_{x\in R_n} f(x)^2} + \frac{2\sum_{\{x,y\}\notin E_1} f(x)f(y)}{\sum_{x\in R_n} f(x)^2} \\
&\leq \lambda_2(A_{\mathcal{P}_n}) + \frac{2\sum_{\{x,y\}\notin E_1} f(x)f(y)}{\sum_{x\in R_n} f(x)^2}
\end{aligned}$$

where the last inequality follows since f is orthogonal to the constant vector $\mathbf{1}$. Using Theorem 4.1.2 we have $\lambda_2(A_{\mathcal{P}_n}) = n - 2$.

To bound the second term, we will partition the edges not in E_1 in the following way

$$\{\{x,y\} \notin E_1\} = E(U_1(1)) \cup E(U_2(1)) \cup \cdots \cup E(U_n(1)).$$

Hence, we have

$$\begin{aligned} \frac{2\sum_{\{x,y\}\notin E_1} f(x)f(y)}{\sum_{x\in R_n} f(x)^2} &= \frac{\sum_{i=1}^n 2\sum_{\{x,y\}\in E(U_i(1))} f(x)f(y)}{\sum_{i=1}^n \sum_{x\in U_i(1)} f(x)^2} \\ &\leq \max_{1\leq i\leq n} \frac{2\sum_{\{x,y\}\in E(U_i(1))} f(x)f(y)}{\sum_{x\in U_i(1)} f(x)^2} \\ &\leq \lambda_2(A_{R_{n-1}}) \end{aligned}$$

where we are using the fact that v sums to zero over each set $U_i(1)$. Combining the two inequalities above, we get

$$\begin{aligned} \lambda &\leq \lambda_2(A_{\mathcal{P}_n}) + \lambda_2(A_{R_{n-1}}) \\ &= (n-2) + \binom{n-1}{2} - (n-1) \\ &= \binom{n}{2} - n \end{aligned}$$

Thus we conclude that $\lambda_2(A_{R_n}) = \binom{n}{2} - n$ and this completes the proof of Theorem 4.1.1. □

4.4 Future work

Consider the stochastic process of pancake flipping: Start with a stack of n pancakes (or n cards). At each step, with probability $1/n$, choose i where $i = 1, \ldots, n$ and do a pancake flipping of the first i pancakes. The above process is equivalent to taking a random walk on $\mathcal{P}_n + I$, where $\mathcal{P}_n$ is the pancake graph. The transition probability matrix is then $P = (A(\mathcal{P}_n) + I)/n$.

Since the first nontrivial eigenvalue of the normalized Laplacian of $\mathcal{P}_n$ is $1/(n-1)$. Consequently, the first nontrivial eigenvalue of the normalized Laplacian of $\mathcal{P}_n + I$ is $1/n$ and all eigenvalues of the normalized Laplacian of $\mathcal{P}_n + I$ are at most $2 - 1/n$. It is known that the rate of convergence for random walk is the inverse of μ^{-1} where $\mu = \min\{\mu_1, 2-\mu_{n-1}\}$ where $0 = \mu_0, \mu_1, \ldots, \mu_{n-1}$ are the nontrivial eigenvalues of the normalized Laplacian of $\mathcal{P}_n + I$. However, in order to get tight bounds for the convergence of the random walk to the stationary distribution under the total variational distance, more work is needed. For a vertex-transitive graph, a general upper bound after t steps of random walk on $\mathcal{P}_n + I$ can be derived by using the Plancherel formula (see [15]):

$$\Delta_{TV}(t) \leq \frac{1}{2}\Big(\sum_{i\neq 0}(1-\mu_i)^{2t}\Big)^{1/2}.$$

Using the result that $|1-\mu_i| \leq 1-1/n$ for $i \neq 0$, we have

$$\begin{aligned}\Delta_{TV}(t) &< \frac{1}{2}\Big(1-\frac{1}{n}\Big)^{t} n! \\ &\leq e^{-t/n+n\log n}.\end{aligned}$$

Hence, the random walk converges to the uniform distribution with $\Delta_{TV}(t) \leq e^{-c}$ after at most $t = n^2 \log n + cn$ steps. If we know more about the distribution of eigenvalues μ_i, this upper bound should be improved. It seems reasonable to conjecture that $O(n\log n)$ steps suffice.

Similarly, we can consider the random substring reversal process, where in each step, with probability $\binom{n+1}{2}^{-1}$ we choose a substring (allowing substrings of length 1) and reverse it. This is equivalent to taking a random walk on $R_n + nI$. In this case, we have $\mu_1 = n/\binom{n+1}{2} = 2(n+1)^{-1}$ and $\mu_{n-1} \leq 2-2(n+1)^{-1}$. As in the case of pancake flipping, knowing the spectral gap allows us to obtain a bound on the rate of convergence, but to obtain sharp bounds it would be desirable to know more about the distribution of all eigenvalues.

We have mainly focused on substring reversal and pancake flipping on permutations. There are many interesting variations of these problems. In particular, for applications such as genome rearrangement, the objects of interest are signed permutations. In this case the operation of substring reversal is taking the reverse of the substring and changing the signs of every element in the substring. The corresponding problem for pancake flipping is the *burnt* pancake problem where the sign is used to distinguish the two sides of each pancake. The burnt pancake graph $\bar{\mathcal{P}}_n$ has $2^n n!$ vertices and degree n. A natural question is to determine the spectral gap of the adjacency matrix. In fact, $\mathcal{P}_n + I$ is a projection of $\bar{\mathcal{P}}_n$, which implies that the adjacency spectral gap of $\bar{\mathcal{P}}_n$ is at least one. A natural guess is that the spectral gap of the adjacency matrix of $\bar{\mathcal{P}}_n$ is exactly 1. However, this turns out to be not true. For $\bar{\mathcal{P}}_4$ the spectral gap is approximately 0.71343, and for $\bar{\mathcal{P}}_5$ the spectral gap is approximately 0.75758.

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