Three conjectures in extremal spectral graph theory

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Abstract

We prove three conjectures regarding the maximization of spectral invariants over certain families of graphs. Our most difficult result is that the join of P_2 and P_{n-2} is the unique graph of maximum spectral radius over all planar graphs. This was conjectured by Boots and Royle in 1991 and independently by Cao and Vince in 1993. Similarly, we prove a conjecture of Cvetković and Rowlinson from 1990 stating that the unique outerplanar graph of maximum spectral radius is the join of a vertex and P_{n-1}. Finally, we prove a conjecture of Aouchiche et al from 2008 stating that a pineapple graph is the unique connected graph maximizing the spectral radius minus the average degree. To prove our theorems, we use the leading eigenvector of a purported extremal graph to deduce structural properties about that graph. Using this setup, we give short proofs of several old results: Mantel's Theorem, Stanley's edge bound and extensions, the Kővari-Sós-Turán Theorem applied to $\mathrm{ex}\,(n, K_{2,t})$, and a partial solution to an old problem of Erdős on making a triangle-free graph bipartite.

1 Introduction

Questions in *extremal graph theory* ask to maximize or minimize a graph invariant over a fixed family of graphs. Perhaps the most well-studied problems in this area are Turán-type problems, which ask to maximize the number of edges in a graph which does not contain fixed forbidden subgraphs. Over a century old, a quintessential example of this kind of result is Mantel's theorem, which states that $K_{\lceil n/2\rceil,\lfloor n/2\rfloor}$ is the unique graph maximizing the number of edges over all triangle-free graphs. *Spectral graph theory* seeks to associate a matrix to a graph and determine graph properties by the eigenvalues and eigenvectors of that matrix. This paper studies the maximization of spectral invariants over various families of graphs. We prove three conjectures.

Conjecture 1 (Boots-Royle 1991 [8] and independently Cao-Vince 1993 [10])**.** *The planar graph on $n \geq 9$ vertices of maximum spectral radius is $P_2 + P_{n-2}$.*

Conjecture 2 (Cvetković-Rowlinson 1990 [13])**.** *The outerplanar graph on n vertices of maximum spectral radius is $K_1 + P_{n-1}$.*

Conjecture 3 (Aouchiche et al 2008 [3])**.** *The connected graph on n vertices that maximizes the spectral radius minus the average degree is a pineapple graph.*

In this paper, we prove Conjectures 1, 2, and 3, with the caveat that we must assume n is large enough in all of our proofs. We note that the Boots-Royle/Vince-Cao conjecture is not true when $n \in \{7, 8\}$ and thus some bound on n is necessary.

For each theorem, the rough structure of our proof is as follows. A lower bound on the invariant of interest is given by the conjectured extremal example. Using this information, we deduce the approximate structure of a (planar, outerplanar, or connected) graph maximizing this invariant. We then use the leading eigenvalue and eigenvector of the adjacency matrix of the graph to deduce structural properties of the extremal graph. Once we know the extremal graph is "close" to the conjectured graph, we show that it must be exactly the conjectured graph.

The majority of the work in each proof is done in the step of using the leading eigenvalue and eigenvector to deduce structural properties of the extremal graph. We choose a normalization of the leading eigenvector which is particularly convenient for our purposes, and using this setup, we give short proofs of the following known results:

- Mantel's Theorem.
- Stanley's Bound [39]: if G is a graph with m edges and λ_1 is the spectral radius of its adjacency matrix, then $\lambda_1 \leq \frac{1}{2}\left(-1 + \sqrt{1+8m}\right)$.
- A long-standing conjecture of Erdős [17] is that every triangle-free graph may be made bipartite with the removal of at most $n^2/25$ edges. We show that the conjecture is true for graphs with at least $n^2/5$ edges, first proved by Erdős, Faudree, Pach, and Spencer [18].
- If G is a $K_{2,t}$-free graph and the spectral radius of its adjacency matrix is λ_1, then $\lambda_1 \leq 1/2 + \sqrt{(t-1)(n-1)+1/4}$. This was originally proved by Nikiforov [34] and is a spectral strengthening of the Kővari-Sós-Turán Theorem applied to $\mathrm{ex}\left(n, K_{2,t}\right)$ [26].
- An improvement of the Stanley Bound [43] and some variants of it when one forbids cycles of length 3 and 4 [31, 37].
- An upper bound on the spectral radius of a graph based on local structure, first proved by Favaron, Mahéo, and Saclé [19].

1.1 History and Motivation

Questions in extremal graph theory ask to maximize or minimize a graph invariant over a fixed family of graphs. This question is deliberately broad, and as such branches into several areas of mathematics. We already mentioned Mantel's Theorem as an example of a theorem in extremal graph theory. Other classic examples include the following. Turán's Theorem [41] seeks to maximize the number of edges over all n-vertex K_r-free graphs. The Four Color Theorem seeks to maximize the chromatic number over the family of planar graphs. Questions about maximum cuts over various families of graphs have been studied extensively (cf [2, 7, 11, 20]). The Erdős distinct distance problem seeks to minimize the number of distinct distances between n points in the plane [16, 22].

This paper studies *spectral extremal graph theory*, the subset of these extremal problems where invariants are based on the eigenvalues or eigenvectors of a graph.

This subset of problems also has a long history of study. Examples include Stanley's bound maximizing spectral radius over the class of graphs on m edges [39], the Alon-Bopanna-Serre Theorem (see [28, 36]) and the construction of Ramanujan graphs (see [27]) minimizing λ_2 over the family of d-regular graphs, theorems of Wilf [42] and Hoffman [24] relating eigenvalues of graphs to their chromatic number, and many other examples. Very recently, Bollobás, Lee, and Letzter studied maximizing the spectral radius of subgraphs of the hypercube on a fixed number of edges [6].

A bulk of the recent work in spectral extremal graph theory is by Nikiforov, who has considered maximizing the spectral radius over several families of graphs. Using the fundamental inequality that $\lambda_1(A(G)) \geq 2e(G)/n$, Nikiforov recovers several classic results in extremal graph theory. Among these are spectral strengthenings of Turán's Theorem [29], the Erdős-Stone-Bollobás Theorem [33], the Kővari-Sós-Turán Theorem regarding the Zarankiewicz problem [34] (this was also worked on by Babai and Guiduli [4]), and the Moore Bound [32]. For many other similar results of Nikiforov, see [35].

We now turn to the history specific to our theorems.

The study of spectral radius of planar graphs has a long history, dating back to at least Schwenk and Wilson [25]. 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. To compare connectivity of networks to a theoretical upper bound, geographers were interested in finding the planar graph of maximum spectral radius. To this end, Boots and Royle and independently Cao and Vince conjectured that the extremal graph is $P_2 + P_{n-2}$ [8], [10]. Several researchers have worked on this problem and successively improved upon the best theoretical upper bound, including [43], [10], [44], [21], [45], [15]. 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 [14]. Work has also been done maximizing the spectral radius of graphs on surfaces of higher genus [15, 44, 45].

Conjecture 2 appears in [13], where they mention that it is related to the study of various subfamilies of Hamiltonian graphs. Rowlinson [38] made partial progress on this conjecture, which was also worked on by Cao and Vince [10] and Zhou-Lin-Hu [46].

Various measures of graph irregularity have been proposed and studied (cf [1, 5, 12, 30] and references therein). These measures capture different aspects of graph irregularity and are incomparable in general. Because of this, a way to understand which graph properties each invariant gauges is to look at the extremal graph. For several of the measures, the graph of maximal irregularity with respect to that measure has been determined [5, 9, 23, 40]. One such invariant is the spectral radius of the graph minus its average degree, and Conjecture 3 proposes that the extremal connected graph is a pineapple graph.

1.2 Notation and Preliminaries

Let G be a connected graph and A the adjacency matrix of G. For sets $X, Y \subset V(G)$ we will let $e(X)$ be the number of edges in the subgraph induced by X and $e(X, Y)$

be the number of edges with one endpoint in X and one endpoint in Y. For a vertex $v \in V(G)$, we will use $N(v)$ to denote the neighborhood of v and d_v to denote the degree of v. For graphs G and H, $G + H$ will denote their join.

Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of A, and let $\mathbf{v}$ be an eigenvector corresponding to λ_1. By the Perron-Frobenius Theorem, $\mathbf{v}$ has all positive entries, and it will be convenient for us to normalize so that the maximum entry is 1. For a vertex $u \in V(G)$, we will overdefine the symbol u to represent both the vertex and the entry of $\mathbf{v}$ corresponding to u. It will be clear from context which meaning we are using. With this notation, for any $u \in V(G)$, the eigenvector equation becomes

$$\lambda_1 u = \sum_{v \sim u} v. \tag{1}$$

Throughout the paper, we will use x to denote the vertex with maximum eigenvector entry equal to 1. If there are multiple such vertices, choose and fix x arbitrarily among them. Since $x = 1$, (1) applied to x becomes

$$\lambda_1 = \sum_{x \sim y} y. \tag{2}$$

Note that this implies $\lambda_1 \leq d_x$. The next inequality is a simple consequence of our normalization and an easy double counting argument, but will be incredibly useful. Multiplying both sides of (2) by λ_1 and applying (1) gives

$$\lambda_1^2 = \sum_{x \sim y} \sum_{z \sim y} z = \sum_{x \sim y} \sum_{\substack{z \sim y \\ z \in N(x)}} z + \sum_{x \sim y} \sum_{\substack{z \sim y \\ z \notin N(x)}} z \leq 2e\left(N(x)\right) + e\left(N(x), V(G) \setminus N(x)\right) \tag{3}$$

where the last inequality follows because each eigenvector entry is at most 1, and because each eigenvector entry appears at the end of a walk of length 2 from x: each edge with both endpoints in $N(x)$ is the second edge of a walk of length 2 from x exactly twice and each edge with only one endpoint in $N(x)$ is the second edge of a walk of length 2 from x exactly once.

We will also use the Rayleigh quotient characterization of λ_1:

$$\lambda_1 = \max_{\mathbf{z} \neq \mathbf{0}} \frac{\mathbf{z}^t A \mathbf{z}}{\mathbf{z}^t \mathbf{z}}. \tag{4}$$

In particular, this definition of λ_1 and the Perron-Frobenius Theorem imply that if H is a strict subgraph of G, then $\lambda_1(A(G)) > \lambda_1(A(H))$. Another consequence of (4) that we use frequently is that $\lambda_1 \geq \frac{2m}{n}$, the average degree of G.

1.3 Outline of the paper

In Section 2, we use (3) to give short proofs of several known results. Section 4 contains our strongest result, the proof of Conjecture 1. In Section 3 we prove Conjecture 2 and in Section 5 we prove Conjecture 3.

2 Short proofs of old results

In this section we prove several known results. Let G be a graph, and as before let $\mathbf{v}$ be an eigenvector for the spectral radius of its adjacency matrix normalized to have maximum entry 1, and let x be a vertex with eigenvector entry equal to 1 (in our notation: $x = 1$). All of our proofs are simple consequences of (3).

Theorem 1 (Mantel's Theorem)**.** *Let G be a triangle-free on n vertices. Then G contains at most $\lfloor n^2/4 \rfloor$ edges. Equality occurs if and only if $G = K_{\lfloor n/2\rfloor \lceil n/2 \rceil}$.*

Proof. If G is triangle-free, then $e(N(x)) = 0$. Using $\lambda_1 \geq \frac{2m}{n}$ and (3) gives

$$\frac{4(e(G))^2}{n^2} \leq e(N(x), V(G) \setminus N(x)) \leq \left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor.$$

Equality may occur only if $e(N(x), V(G) \setminus N(x)) = \lfloor n^2/4 \rfloor$. The only bipartite graph with this many edges is $K_{\lfloor n/2\rfloor \lceil n/2 \rceil}$, and thus $K_{\lfloor n/2\rfloor \lceil n/2 \rceil}$ is a subgraph of G. But G is triangle-free, and so $G = K_{\lfloor n/2\rfloor \lceil n/2 \rceil}$.

□

Theorem 2 (Stanley's Bound [39])**.** *Let G have m edges. Then*

$$\lambda_1 \leq \frac{1}{2}\left(-1 + \sqrt{1+8m}\right).$$

Equality occurs if and only if G is a clique and isolated vertices.

Proof. Using (3) gives

$$\lambda_1^2 = \sum_{x \sim y} \sum_{\substack{y \sim z \\ z \neq x}} z + \sum_{x \sim y} 1 \leq 2(m - d_x) + d_x \leq 2m - \lambda_1,$$

where the last inequality is because $\lambda_1 \leq d_x$. The result follows by the quadratic formula. Examining (3) shows that equality holds if and only if $E(G)$ is contained in the closed neighborhood of x, $d_x = \lambda_1$, and for each $y \sim x$, $y = 1$. Since x was chosen arbitrarily amongst vertices of eigenvector entry 1, any vertex of eigenvector entry 1 must contain $E(G)$ in its closed neighborhood. Thus G is a clique plus isolated vertices. □

Theorem 3 (Erdős-Faudree-Pach-Spencer [18])**.** *Let G be a triangle-free graph on n vertices with at least $n^2/5$ edges. Then G can be made bipartite by removing at most $n^2/25$ edges.*

Proof. Let G be triangle-free with m edges, and let $\mathrm{MaxCut}(G)$ denote the size of a maximum cut in G. So we are trying to show that $m - \mathrm{MaxCut}(G) \leq n^2/25$. Since G is triangle-free, $N(x)$ induces no edges. Thus by (3)

$$\frac{4m^2}{n^2} \leq \lambda_1^2 \leq e(N(x), V(G) \setminus N(x)) \leq \mathrm{MaxCut}(G).$$

Let $g(m) = m - \frac{4m^2}{n^2}$. The function $g(m)$ is decreasing for $m \geq \frac{n^2}{8}$, and $g(n^2/5) = n^2/25$, which implies the result. □

Theorem 4 (Nikiforov [34])**.** *Let G be a $K_{2,t}$-free graph of order n and spectral radius λ_1. Then*

$$\lambda_1 \leq 1/2 + \sqrt{(t-1)(n-1) + 1/4}.$$

Noting that $\lambda_1 \geq \frac{2e(G)}{n}$ implies the Kővari-Sós-Turán Theorem applied to $\mathrm{ex}(n, K_{2,t})$.

Proof. Let z be a vertex not equal to x. Since G is $K_{2,t}$-free, there are at most $t-1$ walks of length 2 from x to z. Therefore, by (3)

$$\begin{aligned}
\lambda_1^2 &= d_x + \sum_{x\sim y} \sum_{\substack{y\sim z \\ z\in N(x)}} z + \sum_{x\sim y} \sum_{\substack{y\sim z \\ z\notin N(x) \\ z\neq x}} z \\
&\leq d_x + (t-1) \sum_{z\in N(x)} z + (t-1) \sum_{\substack{z\notin N(x) \\ z\neq x}} z \\
&= d_x + \sum_{z\in N(x)} z + (t-2) \sum_{z\in N(x)} z + (t-1) \sum_{\substack{z\notin N(x) \\ z\neq x}} z \\
&= d_x + \lambda_1 + (t-2) \sum_{z\in N(x)} z + (t-1) \sum_{\substack{z\notin N(x) \\ z\neq x}} z \\
&\leq d_x + \lambda_1 + (t-2)d_x + (t-1)(n-d_x-1).
\end{aligned}$$

Applying the quadratic formula yields the result. □

The next three theorems are variants of Stanley's edge bound. Theorem 7 implies Stanley's bound.

Theorem 5 (Nosal [37])**.** *If G is triangle free with m edges and spectral radius λ_1, then $\lambda_1 \leq \sqrt{m}$.*

Proof. If G is triangle-free, then $e(N(x)) = 0$. (3) implies

$$\lambda_1^2 \leq e(N(x), V(G) \setminus N(x)) \leq m.$$

□

Theorem 6 (Nikiforov [31])**.** *Let G be an n-vertex graph of girth at least 5 and spectral radius λ_1. Then $\lambda_1 \leq \sqrt{n-1}$.*

Proof. Since G is triangle and quadrilateral-free, $e(N(x)) = 0$ and for any $z \in V(G) \setminus \{x \cup N(x)\}$ $|N(z) \cap N(x)| \leq 1$. Therefore $e(N(x), V(G) \setminus N(x)) \leq d_x + (n - d_x - 1)$. (3) gives $\lambda_1^2 \leq n-1$. □

Using $\lambda_1 \leq \Delta(G)$, we have for G of girth at least 5, $\lambda_1 \leq \min\{\Delta, \sqrt{n-1}\}$. Nikiforov [31] characterizes the cases of equality. We leave the characterization of equality using our proof to the reader.

Theorem 7 (Hong [43])**.** *Let G be a connected graph on m edges with spectral radius λ_1, then*

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

Equality occurs if and only if G is either a complete graph or a star.

Proof. Since G is connected, every vertex in $V(G) \setminus \{x \cup N(x)\}$ has degree at least 1. Therefore, at least $n - d_x - 1$ edges contribute at most 1 to the sum in (3). This gives

$$\lambda_1^2 \leq d_x + 2e(N(x)) - (n - d_x - 1) \leq 2m - n + 1.$$

Equality occurs if and only if for all $u \in V(G) \setminus \{x \cup N(x)\}$, $d_u = 1$ and for any walk of length 2 starting at x and ending at z, $z = 1$. These conditions together imply that $V(G) = x \cup N(x)$. Now, if there are any edges in $N(x)$, then both endpoints must have eigenvector entry 1. If $z = 1$ and $N(z) \subset \{x \cup N(x)\}$, then $N(z)$ must equal $V(G) \setminus \{z\}$. Therefore G is either a clique or a star. □

Finally, we note that some of the above theorems are corollaries of the following bound by Favaron, Mahéo, and Saclé. We prove (a stronger version of) their theorem immediately from (3)

Theorem 8 (Favaron-Mahéo-Saclé [19])**.** *Let G be a graph with spectral radius λ_1. For $i \in V(G)$ let s_i be the sum of the degrees of the vertices adjacent to i. Then*

$$\lambda_1 \leq \max_i \sqrt{s_i}.$$

Proof. Since $2e(N(x)) + e(N(x), V(G) \setminus N(x)) = s_x$, we have immediately from (3)

$$\lambda_1^2 \leq s_x \leq \max_{i \in V(G)} s_i.$$

□

3 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 facts that we will use frequently are that since G is outerplanar, 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 vertex of large degree and that the rest of the vertices have small eigenvector entry (Lemma 11). We use this to show that the vertex of large degree must be connected to every other vertex (Lemma 12). 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 needs.

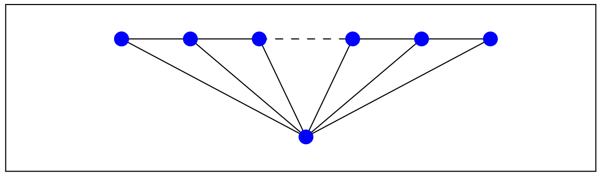

Figure 1: The graph $P_1 + P_{n-1}$.

Lemma 9. $\lambda_1 > \sqrt{n-1}$.

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. By the Rayleigh quotient, $\lambda_1(G) > \lambda_1(K_{1,n}) = \sqrt{n-1}$. $\square$

Lemma 10. *For any vertex u, we have $d_u > un - 12\sqrt{n}$.*

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

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

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

$$\sum_{y\sim u}\sum_{z\in N(y)\cap A} z \leq 2\sum_{y\sim u} y = 2\lambda_1 u$$

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

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

as $e(G) \leq 2n-3$ by outerplanarity. So, for n sufficiently large and using Lemma 9 we have

$$\sum_{y\sim u}\sum_{z\in N(y)\cap B} z < 9\sqrt{n}$$

Combining the above inequalities yields

$$\lambda_1^2 u - 2\lambda_1 u < d_u + 9\sqrt{n}$$

Again using Lemma 9 we get

$$un - 12\sqrt{n} < (n - 1 - 2\sqrt{n-1})u - 9\sqrt{n} < d_u.$$

$\square$

Lemma 11. *We have $d_x > n - 12\sqrt{n}$ and for every other vertex u, $u < C_1/\sqrt{n}$ 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 $x = 1$. Now consider any other vertex u. We know that G contains no $K_{2,3}$, so $d_u < 13\sqrt{n}$, otherwise u, x share $\sqrt{n}$ neighbors, which yields a $K_{2,3}$ if $n \geq 9$. So

$$13\sqrt{n} > d_u > un - 12\sqrt{n},$$

that is, $u < 25/\sqrt{n}$. □

Lemma 12. *Let $B = V(G) \setminus (N(x) \cup \{x\})$. Then*

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

for some absolute constant C_2.

Proof. From the previous lemma, we have that $|B| < 12\sqrt{n}$. Now

$$\sum_{z \in B} z \leq \frac{1}{\lambda_1} \sum_{z \in B} \left(25/\sqrt{n}\right) d_z = \frac{25}{\lambda_1 \sqrt{n}} \left(e(A, B) + 2e(B)\right)$$

Each vertex in B is connected to at most two vertices in A, so $e(A, B) \leq 2|B| < 24\sqrt{n}$. The graph induced on B is outerplanar, so $e(B) \leq 2|B| - 3 < 24\sqrt{n}$. Finally, using the fact that $\lambda_1 > \sqrt{n-1}$, we get the required result. □

Theorem 13. *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, ie x is connected to every other vertex. If not, let $y \in B$. Now y is connected to at most two vertices in B, and so by Lemma 11 and Lemma 12,

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

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

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

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

Now x is connected to every other vertex in G. Hence every other vertex has degree less than or equal to 2. It follows that G is a subgraph of $K_1 + P_{n-1}$, and maximality ensures that G must be equal to $K_1 + P_{n-1}$. □

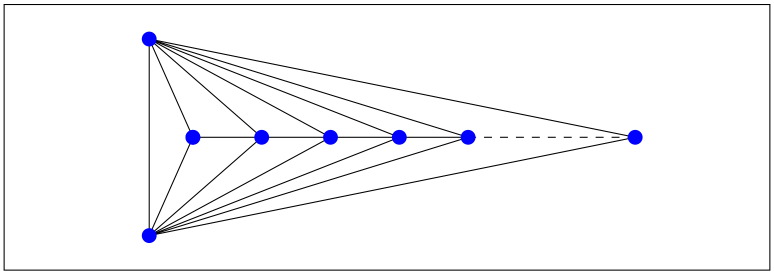

Figure 2: The graph $P_2 + P_{n-2}$.

4 Planar graphs of maximum spectral radius

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 connected to most of the rest of the graph (Lemmas 14–17). We then show that the two vertices of large degree are adjacent (Lemma 19), and that they are connected to every other vertex (Lemma 20). The proof of the theorem follows readily.

Lemma 14. $\lambda_1 > \sqrt{2n-4}$.

Proof. 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,

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

□

Next we partition the graph into vertices of small eigenvector entry and those with large eigenvector entry. Let

$$L := \{z \in V(G) : z > \epsilon\}$$

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

$$6n - 12 \geq \sum_{z \in V(G)} d_z \geq \sum_{z \in L} d_z \geq |L|\epsilon\sqrt{2n-4},$$

yielding $|L| \leq \frac{3\sqrt{2n-4}}{\epsilon}$. 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 $e(L) \leq \frac{9\sqrt{2n-4}}{\epsilon}$.

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 15.

$$\sum_{z\in L} z \leq \epsilon\sqrt{2n-4} + \frac{18}{\epsilon} \tag{5}$$

and

$$\sum_{z\in S} z \leq (1+3\epsilon)\sqrt{2n-4} \tag{6}$$

Proof.

$$\sum_{z\in L} \lambda_1 z = \sum_{z\in L}\sum_{y\sim z} y = \sum_{z\in L}\sum_{\substack{y\sim z\\ y\in S}} y + \sum_{\substack{y\sim z\\ y\in L}} y \leq \epsilon e(S,L) + 2e(L) \leq \epsilon(2n-4) + \frac{18\sqrt{2n-4}}{\epsilon}.$$

Dividing both sides by λ_1 and using Lemma 14 gives (5).

On the other hand,

$$\sum_{z\in S} \lambda_1 z = \sum_{z\in S}\sum_{y\sim z} y \leq 2\epsilon e(S) + e(S,L) \leq (6n-12)\epsilon + (2n-4).$$

Dividing both sides by λ_1 and using Lemma 14 gives (6). □

Now let $u \in L$

$$u\sqrt{2n-4} \leq \lambda_1 u = \sum_{y\sim u} y = \sum_{\substack{y\sim u\\ y\in L}} y + \sum_{\substack{y\sim u\\ y\in S}} y \leq \sum_{y\in L} y + \sum_{\substack{y\sim u\\ y\in S}} y.$$

By (5), this gives

$$\sum_{\substack{y\sim u\\ y\in S}} y \geq (u-\epsilon)\sqrt{2n-4} - \frac{18}{\epsilon}. \tag{7}$$

The equations (6) and (7) imply that if $u \in L$ and u is close to 1, then the sum of the eigenvector entries of vertices in S not adjacent to u is small. To conclude that this implies u is connected to most vertices in S we need the following lemma.

Lemma 16. *For all z we have $z > \frac{1}{\sqrt{2n-4}}$.*

Proof. By way of contradiction assume $z \leq \frac{1}{\sqrt{2n-4}}$. By the eigenvector equation z cannot be adjacent to x. Let H be the graph obtained from G by removing all edges incident with z and making z adjacent to x. By the Rayleigh quotient, we have $\lambda_1(H) > \lambda_1(G)$, a contradiction. □

Now letting $u = x$ and combining (7) and (6) gives

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

Now applying Lemma 16 gives

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

For n large enough, we have $|\{y \in S : y \not\sim x\}| \leq 9\epsilon n$. 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 17. *There is a $w \in L$ with $w \neq x$ such that $w > 1 - 20\epsilon$ and $|\{y \in S : y \not\sim w\}| \leq 49\epsilon n$.*

Proof. By the eigenvector equation, we see

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

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

$$2n-4 \leq \lambda_1^2 + \lambda_1 \leq \sum_{uv\in E(G)} u+v = \left(\sum_{uv\in E(S,L)} u+v\right) + \left(\sum_{uv\in E(S)} u+v\right) + \left(\sum_{uv\in E(L)} u+v\right)$$
$$\leq \left(\sum_{uv\in E(S,L)} u+v\right) + \epsilon(6n-12) + \frac{18\sqrt{2n-4}}{\epsilon}.$$

So for n large enough,

$$(2-7\epsilon)n \leq \sum_{uv\in E(S,L)} u+v = \left(\sum_{\substack{uv\in E(S,L)\\ u=x}} u+v\right) + \left(\sum_{\substack{uv\in E(S,L)\\ u\neq x}} u+v\right) \leq \epsilon e(S,L) + d_x + \sum_{\substack{uv\in E(S,L)\\ u\neq x}} u$$

giving

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

Now since $d_x \geq |S| - 9\epsilon n > (1-10\epsilon)n$, and $e(S,L) < 2n$, the number of terms in the left hand side of the sum is at most $(1+10\epsilon)n$. By averaging, there is a $w \in L$ such that

$$w > \frac{1-9\epsilon}{1+10\epsilon} > 1-20\epsilon,$$

for ϵ small enough. Applying (7) and (6) to this w gives

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

and applying Lemma 16 gives that for n large enough

$$|\{y \in S : y \not\sim w\}| \leq 49\epsilon n$$

for n large enough.

$\square$

For the rest of the section, let w be the vertex from Lemma 17. So $x = 1$ and $w > 1 - 20\epsilon$, and both are connected to most of S. Our next goal is to show that all of the remaining vertices are connected 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 18. *Let $v \in V(G) \setminus \{x, w\}$. Then $v < \frac{1}{10}$.*

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 connected to at most one of x and w, and is connected to at most 2 vertices in B (otherwise G would contain a $K_{3,3}$ and would not be planar). Thus

$$\lambda_1 \sum_{v\in A} v \leq \sum_{v\in A} d_v \leq 3|A| + 2e(A) \leq 9|A|,$$

where the last inequality is using that $e(A) \leq 3|A|$ since A induces a planar graph. Now, since $|L| < \frac{3\sqrt{2n-4}}{\epsilon} < 1\epsilon n$ for n large enough, we have $|A| \leq (9 + 49 + 1)\epsilon n$ (by Lemma 17) . Therefore

$$\sum_{v\in A} v \leq \frac{9 \cdot 59 \cdot \epsilon n}{\sqrt{2n-4}}.$$

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

$$\lambda_1 v = \sum_{u\sim v} u \leq 4 + \sum_{\substack{u\sim v\\ u\in A}} u \leq 4 + \sum_{u\in A} u \leq C\epsilon\sqrt{n}$$

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

We use the fact that the eigenvector entries in A are small to show that if $v \in A$ (ie v is not connected to both x and w), then removing all edges from v and connecting it to x and w increases the spectral radius, showing that A must be empty. To do this, we must be able to connect a vertex to both x and w and have the resulting graph remain planar. This is accomplished by the following lemma.

Lemma 19. *If G is extremal, then $x \sim w$.*

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

Proof of Lemma 19. 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. 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 F_1. Let $F = F_1 \cup F_2$. We have that $|F_1| \geq (1-\delta)n$. Now each face in F_1 shares an edge with exactly three other faces. 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 18, 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. $\square$

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

Lemma 20. *A is empty.*

Proof. By way of contradiction, assume 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 19, H

is a planar graph. Then

$$
\begin{aligned}
\mathbf{v}^T\mathbf{v}\lambda_1(H) &\geq \mathbf{v}^T A(H)\mathbf{v} \\
&= \mathbf{v}^T A(G)\mathbf{v} - 2\sum_{z\sim v} vz + 2v(w+x) \\
&\geq \mathbf{v}^T A(G)\mathbf{v} - 14\cdot v\cdot\frac{1}{10} - 2\sum_{\substack{z\sim v\\ z\in\{w,x\}}} vz + 2v(w+x) && \text{(by Lemma 18)} \\
&\geq \mathbf{v}^T A(G)\mathbf{v} - v + 2vw && (|N(v)\cap\{x,w\}|\leq 1) \\
&> \mathbf{v}^T A(G)\mathbf{v} && (\text{as } w > 7/10) \\
&= \mathbf{v}^T\mathbf{v}\lambda_1(G).
\end{aligned}
$$

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

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

Theorem 21. *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 19 and 20, we have that 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 $G = K_2 + P_{n-2}$. □

5 Connected graphs of maximum irregularity

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 22). Then we show that there exists a vertex adjacent to x with degree close to $\frac{n}{2}$ and eigenvector entry close to 1 (Lemmas 23 and 24). 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 25 and Proposition 26). We complete the proof by showing that all vertices not in the clique have degree 1 and that they are all connected to the same vertex.

Lemma 22. *We have $\lambda_1(H) = \frac{n}{2} + c_1\sqrt{n}$ and $\frac{2e(H)}{n} = \frac{n}{4} + c_2\sqrt{n}$, where $|c_1|, |c_2| < 1$.*

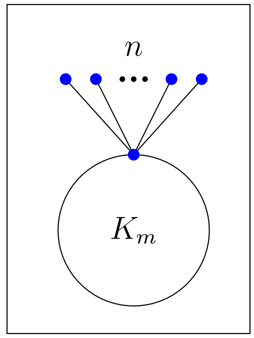

Figure 3: A pineapple graph.

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

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

On the other hand, the eigenvector equation gives

$$\lambda_1^2 = \sum_{y\sim x} \lambda_1 y = \sum_{y\sim x}\sum_{z\sim y} z \leq \sum_{y\sim x} d_y \leq 2e(G) - (n-1),$$

where the last inequality follows because G is connected. This gives

$$d \geq \frac{\lambda_1^2}{n} + 1 - \frac{1}{n}. \tag{8}$$

Setting $\lambda_1 = pn$ and applying (8), 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

$$\frac{n}{4} - \frac{3}{2} \leq \lambda_1 - d \leq \frac{n}{4} - 1 + \frac{1}{n}. \tag{9}$$

Next setting $\lambda_1 = \frac{n}{2} + c_1\sqrt{n}$, (8) gives

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

whereas (9) gives

$$d \leq \lambda_1 - \frac{n}{4} + \frac{3}{2} = \frac{n}{4} + c_1\sqrt{n} + \frac{3}{2}. \tag{10}$$

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

Lemma 23. *There exists a constant c_3 not depending on n such that*

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

Proof. By the eigenvector equation

$$\sum_{y\sim x}\lambda_1 y = \lambda_1^2 = \sum_{y\sim x}\sum_{z\sim y} z \le \sum_{y\sim x} d_y \le dn-(n-1).$$

Rearranging and applying Lemma 22, we have

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

By the eigenvector equation again, and because the first eigenvector is normalized with $x=1$, we have

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

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

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

where the implied constant is independent of n. □

Now we fix a constant $\epsilon > 0$, 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 24. *There exists a vertex $u \ne x$ with $u > 1-2\epsilon$ and $d_u - \lambda_1 u = O(\sqrt{n})$. Moreover $d_u \ge \left(1/2 - 2\epsilon - 4n^{-1/2}\right)n$.*

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

Let $A := \{z \sim x : z > \frac{1}{2} - \epsilon\}$. By Lemma 22,

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

where $|c_1| < 1$. Since $0 < z \le 1$ for all $z \sim x$, we have that $|A| \ge \delta_\epsilon n$ where δ_ϵ is a positive constant that depends only on ϵ. Let $B = \{z \sim x : d_z - \lambda_1 z > K\sqrt{n}\}$. Now

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

By Lemma 23, $|B| \le \frac{c_3}{K}n$. Therefore, for K a large enough constant 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 $U \subset N(y)$ such that $|U| \ge \left(\frac{1}{4}-2\epsilon\right)n$ and $u \ge 1-2\epsilon$ for $u \in U$. By Lemma 22,

$$\left(\frac{n}{2}+c_1\sqrt{n}\right)\left(\frac{1}{2}-\epsilon\right) \le \lambda_1 y \le d_y,$$

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

$$K_\epsilon \sqrt{n} \geq d_y - \lambda_1 y = \sum_{z \sim y} 1 - z \geq \sum_{z \in C} 1 - z \geq 2|C|\epsilon.$$

Therefore

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

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

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

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

Rearranging this we get

$$\bar{d} - \frac{\lambda_1^2}{n} \geq \frac{1}{n} \sum_{y \in U \setminus N(x)} d_y$$

Now applying the bound on $\bar{d}$ from equation 10 yields

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

which implies that

$$\frac{5}{2} n \geq \left(\frac{3}{2} + c_1^2\right) n \geq \sum_{y \in U \setminus N(x)} d_y \geq |U \setminus N(x)|(1-2\epsilon)\lambda_1.$$

So

$$|U \setminus N(x)| \leq \frac{5}{2(1-2\epsilon)} \frac{n}{\lambda_1} \leq \frac{5}{2(1-2\epsilon)} \frac{1}{1/2 + c_1 n^{-1/2}}.$$

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

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 $d_u - \lambda_1 u = O(\sqrt{n})$. Finally

$$d_u \geq u\lambda_1 \geq (1-2\epsilon)(n/2 + c_1\sqrt{n}) \geq \left(1/2 - 2\epsilon - 4n^{-1/2}\right) n.$$

□

Lemma 25. *Let x, y be two vertices in G. If $xy > 1/2 + n^{-1/2} + 6n^{-1}$, then x and y are adjacent. On the other hand, if $xy < 1/2 - 3\epsilon$ 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

$$\frac{n}{2} + \sqrt{n} + 6 \geq \mathbf{v}^t \mathbf{v} > \frac{n}{2} - 2\epsilon n - O(\sqrt{n}) \tag{11}$$

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

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

By Lemma 24, we then have

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

For the upper bound of inequality (11), first set $C = (N(x)\cup\{x\})^C$. Then

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

From the proof of Lemma 24 we have the bound

$$\sum_{z\in C} d_z \leq \frac{5}{2}n.$$

Hence

$$\mathbf{v}^t\mathbf{v} \leq 1 + \frac{n}{2} + c_1\sqrt{n} + \frac{5}{2}\cdot\frac{1}{1/2 + c_1 n^{-1/2}} \leq \frac{n}{2} + \sqrt{n} + 6.$$

This completes the proof of inequality (11).

Let λ_1^+ be the leading eigenvalue of the graph formed by adding the edge $\{x, y\}$ to G. Then by (4) we have

$$\lambda_1^+ - \lambda_1 \geq \frac{\mathbf{v}^t(A^+ - A)\mathbf{v}}{\mathbf{v}^t\mathbf{v}} \geq \frac{2xy}{\mathbf{v}^t\mathbf{v}} \geq \frac{2xy}{n/2 + \sqrt{n} + 6} = \frac{4xy}{n(1 + 2n^{-1/2} + 12n^{-1})}.$$

If $xy > 1/2 + n^{-1/2} + 6n^{-1}$, then

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

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

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

$$\lambda_1 - \lambda_1^- \leq \frac{\mathbf{v}^t(A - A^-)\mathbf{v}}{\mathbf{v}^t\mathbf{v}} \leq \frac{2xy}{n/2 - 2\epsilon n - O(\sqrt{n})} \leq \frac{2xy}{(1/2 - 3\epsilon)n}$$

when n is large enough. Now if $xy < 1/2 - 3\epsilon$, then

$$(\lambda_1 - \bar{d}) - (\lambda_1^- - d^-) < 0.$$

$\square$

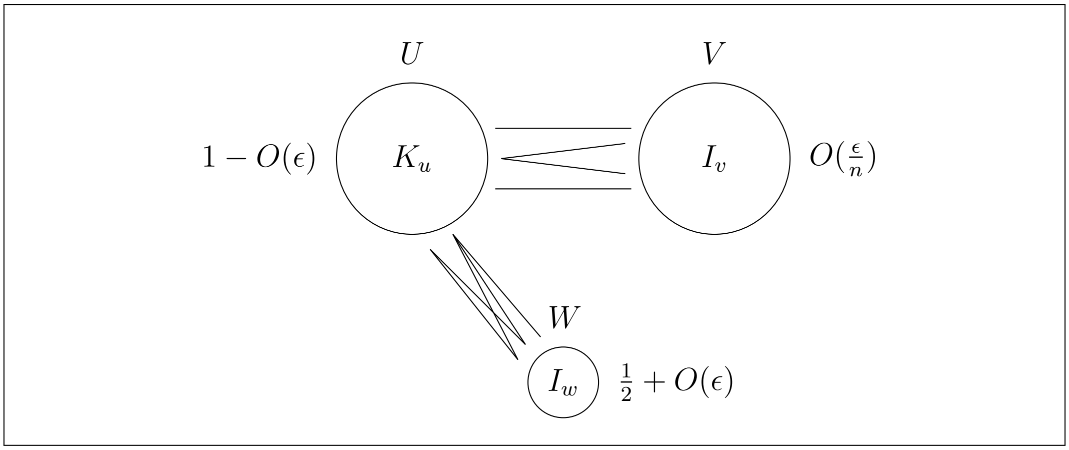

Figure 4: Structure of G_n in Proposition 26. The number appearing beside each set indicates the values of eigenvector entries within the set. U induces a complete graph and V, W induces a independent graphs. Each vertex in V is adjacent to exactly on vertex in U, and each vertex in W is adjacent to multiple vertices in U.

Proposition 26. *For n sufficiently large, we can partition the vertices of G into three sets U, V, W (see Figure 4) where*

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

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

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

Proof.

(i) Let V consist of all vertices in U with eigenvector entry less than $1/2 - 4\epsilon$. By Lemma 25, removing any edge incident to a vertex in U strictly increases $\lambda_1 - d$, so each vertex in U has degree one. By the eigenvector equation, the eigenvector entry of any such vertex is at most $1/\lambda_1 < (2+\epsilon)/n$, when n is large enough.

(ii) From Lemma 24, we have a vertex u such that $d_u - \lambda_1 u = O(\sqrt{n})$. Let X be the set of neighbors x of u such that $x < 9/10$. Then we have

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

Hence $|X| = O(\sqrt{n})$. Let U be all vertices in G with eigenvector entry at least $9/10$. So, by Lemma 24

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

For n large enough, we have $|U| \geq (1/2 - 3\epsilon)n$. For sufficiently large n, by Lemma 25 these vertices are all connected to each other. For the upper bound on $|U|$ we use the expression for $e(G)$ in Lemma 22

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

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

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

$$\lambda_1 - \lambda_1 y \leq \sum_{z \in N(x)\setminus N(y)} z \leq \sum_{z \in V} z + \sum_{z \in W} z \tag{12}$$

From part (i) we have

$$\sum_{z \in W} z < n\,(2+\epsilon)\,/n = (2+\epsilon)$$

For the other term, we have

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

for n sufficiently large, where we are using the expression for $e(G)$ given by Lemma 22. In particular,

$$\sum_{z \in V} z \leq 9\epsilon n$$

Finally, by equation 12 we have

$$y \geq 1 - \frac{1}{\lambda_1} \sum_{z \in V} z - \frac{1}{\lambda_1} \sum_{z \in W} z \geq (1 - 20\epsilon).$$

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

$$(1/2 + 21\epsilon)(1/2 - 20\epsilon) > 1/2 + \epsilon/3$$

and for sufficiently large n by Lemma 25 we have that z is connected to every vertex in U. But by the proof of part (ii), this implies that $z > 1 - 20\epsilon$, which contradicts $z \in W$.

For $z \in W$ and any vertex $y \in U^C$, then $yz \leq (1/2 + 21\epsilon)(1/2 + 21\epsilon) < 1/4 + 22\epsilon$ and so by Lemma 25 there is no edge between y and z in the maximal graph G.

□

Theorem 27. *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. Assume to the contrary, and let z be in W, and 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 connected only to vertices in U, and the fact that vertices in U have eigenvector entry between $1 - 20\epsilon$ and 1, the eigenvector equation yields

$$\lambda_1(1/2 - 4\epsilon) \leq \lambda_1 z \leq e(z, U) \leq \frac{\lambda_1 z}{1 - 20\epsilon} = (1/2 + O(\epsilon))\lambda_1$$

Using the expression for λ_1 in Lemma 22, for large enough n we have

$$(1 - \epsilon)\,\frac{n}{4} \leq e(z, U) \leq (1 + \epsilon)\,\frac{n}{4}$$

So we can bound the change in the average degrees

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

Next we find a lower bound on $\lambda_1(G^+) - \lambda_1(G)$. If $\mathbf{v}$ is the leading eigenvector of $A(G)$, normalized so that $||\mathbf{v}||_\infty = 1$, 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)

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

Similarly, we find an upper bound for the denominator

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

Combining these, and using the bound on $\mathbf{v}^t \mathbf{v}$ from the proof of Lemma 25, we get

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

Hence $\lambda_1(G^+) - \lambda_1(G) > d(G^+) - d(G)$, and from Lemma 25 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 connected to. Let x be a vertex in G with eigenvector entry 1. Let G^+ be the graph obtained from G by deleting the edges $\{v_i, u_i\}$ and adding the edges $\{v_i, x\}$. Now, $d(G^+) = d(G)$, and

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

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

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

with equality if and only if $u_i = 1$ 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 eigenvector entry 1. It follows that the vertices in V are all connected to a single vertex in U, and hence G is a pineapple graph.

□

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